

Phenanthrene

Other names:	Phenanthren Phenanthrin Phenantrin
Inchi:	InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H
InchiKey:	YNPNZTXNASCQKK-UHFFFAOYSA-N
Formula:	C14H10
SMILES:	c1ccc2c(c1)ccc1ccccc12
Mol. weight [g/mol]:	178.23
CAS:	85-01-8

Physical Properties

Property code	Value	Unit	Source
affp	820.10	kJ/mol	NIST Webbook
affp	825.70	kJ/mol	NIST Webbook
basg	795.00	kJ/mol	NIST Webbook
basg	793.70	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
ea	-0.01 ± 0.04	eV	NIST Webbook
ea	0.20	eV	NIST Webbook
ea	0.31 ± 0.01	eV	NIST Webbook
ea	0.27 ± 0.04	eV	NIST Webbook
gf	383.08	kJ/mol	Joback Method
hf	203.80	kJ/mol	NIST Webbook
hf	201.20 ± 4.70	kJ/mol	NIST Webbook
hf	206.90 ± 4.60	kJ/mol	NIST Webbook
hf	202.20 ± 2.30	kJ/mol	NIST Webbook
hf	163.60	kJ/mol	NIST Webbook
hfs	116.10 ± 1.40	kJ/mol	NIST Webbook
hfs	72.80 ± 2.60	kJ/mol	NIST Webbook
hfs	110.10 ± 2.20	kJ/mol	NIST Webbook
hfs	113.00	kJ/mol	NIST Webbook
hfs	109.80 ± 1.60	kJ/mol	NIST Webbook
hfus	15.15	kJ/mol	Thermodynamic study of (anthracene + phenanthrene) solid state mixtures
hvap	79.00 ± 1.20	kJ/mol	NIST Webbook
hvap	78.70	kJ/mol	NIST Webbook

hvap	78.50	kJ/mol	NIST Webbook
hvap	78.70	kJ/mol	NIST Webbook
ie	7.89 ± 0.05	eV	NIST Webbook
ie	7.89 ± 0.00	eV	NIST Webbook
ie	7.87 ± 0.02	eV	NIST Webbook
ie	7.75	eV	NIST Webbook
ie	8.03 ± 0.01	eV	NIST Webbook
ie	7.91 ± 0.01	eV	NIST Webbook
ie	8.03 ± 0.01	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	8.22	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
ie	8.03	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	8.03	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
ie	7.91	eV	NIST Webbook
ie	7.85	eV	NIST Webbook
ie	7.86 ± 0.02	eV	NIST Webbook
ie	7.86	eV	NIST Webbook
ie	7.87 ± 0.02	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.89 ± 0.00	eV	NIST Webbook
ie	23.10	eV	NIST Webbook
ie	7.86 ± 0.01	eV	NIST Webbook
ie	7.92 ± 0.05	eV	NIST Webbook
ie	7.86	eV	NIST Webbook
ie	8.08	eV	NIST Webbook
ie	7.69	eV	NIST Webbook
ie	8.10 ± 0.04	eV	NIST Webbook
ie	7.92 ± 0.02	eV	NIST Webbook
log10ws	-5.26		Estimated Solubility Method
log10ws	-5.26		Aqueous Solubility Prediction Method
logp	3.993		Crippen Method
mcvol	145.440	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1767.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1751.00		NIST Webbook

rinpol	1769.00	NIST Webbook
rinpol	1793.00	NIST Webbook
rinpol	1792.00	NIST Webbook
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rinpol	1778.60	NIST Webbook
rinpol	1786.00	NIST Webbook
rinpol	1759.60	NIST Webbook
rinpol	1778.40	NIST Webbook
rinpol	1790.10	NIST Webbook

rinpol	1776.30	NIST Webbook
rinpol	1776.30	NIST Webbook
rinpol	1756.90	NIST Webbook
rinpol	1776.30	NIST Webbook
rinpol	1789.20	NIST Webbook
rinpol	1769.70	NIST Webbook
rinpol	1791.20	NIST Webbook
rinpol	1797.00	NIST Webbook
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rinpol	1734.95	NIST Webbook
rinpol	1741.00	NIST Webbook
rinpol	1744.37	NIST Webbook
rinpol	1784.21	NIST Webbook
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rinpol	1761.00	NIST Webbook
rinpol	1749.00	NIST Webbook
rinpol	1739.00	NIST Webbook
rinpol	1775.00	NIST Webbook

ripol	2722.00		NIST Webbook
ripol	2712.00		NIST Webbook
ripol	2722.00		NIST Webbook
ripol	2723.00		NIST Webbook
ss	211.70	J/mol×K	NIST Webbook
ss	215.06	J/mol×K	NIST Webbook
tb	609.20	K	NIST Webbook
tb	613.20	K	NIST Webbook
tb	605.15 ± 5.00	K	NIST Webbook
tb	601.15 ± 3.00	K	NIST Webbook
tb	613.15 ± 2.00	K	NIST Webbook
tb	613.00	K	KDB
tc	893.00	K	Critical point measurement of some polycyclic aromatic hydrocarbons
tc	869.00	K	KDB
tc	869.30 ± 1.00	K	NIST Webbook
tc	869.00 ± 1.00	K	NIST Webbook
tf	372.60 ± 0.30	K	NIST Webbook
tf	372.32 ± 0.20	K	NIST Webbook
tf	372.11 ± 0.50	K	NIST Webbook
tf	374.00 ± 1.50	K	NIST Webbook
tf	372.05 ± 1.00	K	NIST Webbook
tf	373.00 ± 2.50	K	NIST Webbook
tf	372.70 ± 1.00	K	NIST Webbook
tf	371.90 ± 0.70	K	NIST Webbook
tf	371.20 ± 1.50	K	NIST Webbook
tf	372.77 ± 0.20	K	NIST Webbook
tf	373.15 ± 0.30	K	NIST Webbook
tf	371.30 ± 1.00	K	NIST Webbook
tf	372.30 ± 0.10	K	NIST Webbook
tf	373.15 ± 1.00	K	NIST Webbook
tf	373.00 ± 2.00	K	NIST Webbook
tf	372.00 ± 1.50	K	NIST Webbook
tf	370.00 ± 1.50	K	NIST Webbook
tf	372.74 ± 0.20	K	NIST Webbook
tf	645.70 ± 0.40	K	NIST Webbook
tf	378.07	K	Solubility of Phenanthrene in Binary Mixtures of C1-C4 Alcohols + 2-Propanol and Ethanol + Methanol at 298.15 K
tf	372.39	K	KDB
tf	372.71	K	Aqueous Solubility Prediction Method
tf	372.90 ± 0.50	K	NIST Webbook
tf	373.00 ± 1.50	K	NIST Webbook

tf	371.40 ± 0.20	K	NIST Webbook
tf	374.20 ± 1.00	K	NIST Webbook
tf	373.00 ± 0.50	K	NIST Webbook
tf	371.70 ± 0.10	K	NIST Webbook
tf	371.40 ± 1.50	K	NIST Webbook
tf	369.50 ± 1.00	K	NIST Webbook
tf	371.15 ± 0.50	K	NIST Webbook
tf	378.65 ± 2.00	K	NIST Webbook
tf	372.95 ± 0.30	K	NIST Webbook
tf	418.00 ± 8.36	K	NIST Webbook
tf	369.40 ± 0.50	K	NIST Webbook
tf	371.80 ± 2.00	K	NIST Webbook
tf	372.80 ± 0.30	K	NIST Webbook
tf	374.15 ± 3.00	K	NIST Webbook
tt	339.52	K	Ternary phase diagram of phenanthrene and carbazole in different solvents and its application in the separation of them
tt	372.38 ± 0.02	K	NIST Webbook
tt	372.38 ± 0.02	K	NIST Webbook
vc	0.554	m3/kmol	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.16	J/mol×K	589.34	Joback Method
cpg	406.65	J/mol×K	843.18	Joback Method
cpg	375.10	J/mol×K	716.26	Joback Method
cpg	362.69	J/mol×K	673.95	Joback Method
cpg	349.09	J/mol×K	631.65	Joback Method
cpg	386.47	J/mol×K	758.56	Joback Method
cpg	396.94	J/mol×K	800.87	Joback Method
cps	134.70	J/mol×K	298.15	NIST Webbook
cps	220.62	J/mol×K	298.15	NIST Webbook
cps	267.40	J/mol×K	343.00	NIST Webbook
cps	220.30	J/mol×K	298.15	NIST Webbook
cps	207.10	J/mol×K	298.10	NIST Webbook
cps	226.40	J/mol×K	298.10	NIST Webbook
cps	233.50	J/mol×K	297.50	NIST Webbook
dvisc	0.0006112	Pa×s	510.19	Joback Method
dvisc	0.0011180	Pa×s	391.46	Joback Method

dvisc	0.0008810	Pa×s	431.03	Joback Method
dvisc	0.0004678	Pa×s	589.34	Joback Method
dvisc	0.0014969	Pa×s	351.88	Joback Method
dvisc	0.0007226	Pa×s	470.61	Joback Method
dvisc	0.0005296	Pa×s	549.76	Joback Method
hfust	16.60	kJ/mol	368.00	NIST Webbook
hfust	17.14	kJ/mol	371.70	NIST Webbook
hfust	17.15	kJ/mol	371.40	NIST Webbook
hfust	16.46	kJ/mol	372.40	NIST Webbook
hfust	18.00	kJ/mol	373.20	NIST Webbook
hfust	18.63	kJ/mol	373.00	NIST Webbook
hfust	15.72	kJ/mol	373.81	NIST Webbook
hfust	16.20	kJ/mol	372.90	NIST Webbook
hsubt	91.60 ± 0.40	kJ/mol	323.00	NIST Webbook
hsubt	95.00 ± 4.40	kJ/mol	318.00	NIST Webbook
hsubt	90.70 ± 1.20	kJ/mol	315.00	NIST Webbook
hsubt	90.90	kJ/mol	298.15	NIST Webbook
hsubt	82.00 ± 2.00	kJ/mol	339.50	NIST Webbook
hsubt	84.10 ± 0.80	kJ/mol	323.00	NIST Webbook
hsubt	84.10 ± 0.80	kJ/mol	313.00	NIST Webbook
hsubt	84.10	kJ/mol	293.00	NIST Webbook
hsubt	81.60	kJ/mol	323.00	NIST Webbook
hsubt	88.90	kJ/mol	383.00	NIST Webbook
hsubt	86.61	kJ/mol	309.70	NIST Webbook
hsubt	86.60	kJ/mol	316.50	NIST Webbook
hsubt	95.80 ± 2.90	kJ/mol	213.00	NIST Webbook
hsubt	96.20	kJ/mol	335.50	NIST Webbook
hsubt	84.10 ± 2.50	kJ/mol	297.00	NIST Webbook
hsubt	87.20	kJ/mol	372.00	NIST Webbook
hsubt	87.20	kJ/mol	344.50	NIST Webbook
hsubt	95.00 ± 0.60	kJ/mol	303.00	NIST Webbook
hsubt	87.20 ± 1.10	kJ/mol	350.00	NIST Webbook
hsubt	95.90	kJ/mol	303.00	NIST Webbook
hvapt	58.20	kJ/mol	502.00	NIST Webbook
hvapt	78.65	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects

hvapt	71.20	kJ/mol	386.00	Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins
hvapt	87.24	kJ/mol	350.00	NIST Webbook
hvapt	72.20	kJ/mol	398.00	NIST Webbook
hvapt	71.20	kJ/mol	398.00	NIST Webbook
hvapt	61.20	kJ/mol	559.50	NIST Webbook
hvapt	69.60	kJ/mol	398.00	NIST Webbook
hvapt	71.20	kJ/mol	372.00	NIST Webbook
hvapt	69.70	kJ/mol	390.00	NIST Webbook
hvapt	67.50	kJ/mol	420.00	NIST Webbook
hvapt	57.20	kJ/mol	548.00	NIST Webbook
hvapt	61.20	kJ/mol	548.00	NIST Webbook
hvapt	59.30	kJ/mol	559.50	NIST Webbook
psub	6.70e-04	kPa	329.47	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.40e-05	kPa	295.73	Development and test of a new Knudsen effusion apparatus for the measurement of low vapour pressures
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psub	8.25e-04	kPa	331.42	The design, construction, and testing of a new Knudsen effusion apparatus

psub	8.14e-04	kPa	331.42	The design, construction, and testing of a new Knudsen effusion apparatus
psub	6.78e-04	kPa	329.47	The design, construction, and testing of a new Knudsen effusion apparatus
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psub	5.44e-04	kPa	327.47	The design, construction, and testing of a new Knudsen effusion apparatus
psub	5.43e-04	kPa	327.47	The design, construction, and testing of a new Knudsen effusion apparatus
psub	4.53e-04	kPa	325.46	The design, construction, and testing of a new Knudsen effusion apparatus
psub	4.46e-04	kPa	325.46	The design, construction, and testing of a new Knudsen effusion apparatus
psub	4.36e-04	kPa	325.46	The design, construction, and testing of a new Knudsen effusion apparatus
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psub	2.96e-04	kPa	321.48	The design, construction, and testing of a new Knudsen effusion apparatus
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psub	2.92e-04	kPa	321.48	The design, construction, and testing of a new Knudsen effusion apparatus
psub	2.39e-04	kPa	319.47	The design, construction, and testing of a new Knudsen effusion apparatus
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psub	1.56e-04	kPa	315.48	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.55e-04	kPa	315.48	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.51e-04	kPa	315.48	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.24e-04	kPa	313.46	The design, construction, and testing of a new Knudsen effusion apparatus
psub	1.50e-05	kPa	295.73	Development and test of a new Knudsen effusion apparatus for the measurement of low vapour pressures
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psub	9.38e-04	kPa	332.95	Development and test of a new Knudsen effusion apparatus for the measurement of low vapour pressures
psub	1.24e-04	kPa	313.46	The design, construction, and testing of a new Knudsen effusion apparatus

psub	1.23e-04	kPa	313.46	The design, construction, and testing of a new Knudsen effusion apparatus
psub	9.58e-04	kPa	332.95	Development and test of a new Knudsen effusion apparatus for the measurement of low vapour pressures
pvap	1.82	kPa	460.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.14	kPa	400.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.18	kPa	404.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.18	kPa	405.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.22	kPa	410.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.27	kPa	415.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	0.34	kPa	420.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.35	kPa	420.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.29	kPa	416.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.24	kPa	412.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.21	kPa	408.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.15	kPa	400.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry

pvap	0.11	kPa	396.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.10	kPa	392.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.08	kPa	388.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	0.06	kPa	384.00	Enthalpies of fusion, vaporisation and sublimation of crown ethers determined by thermogravimetry and differential scanning calorimetry
pvap	3.82	kPa	480.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	3.20	kPa	475.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	2.66	kPa	470.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	2.21	kPa	465.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.42	kPa	425.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.50	kPa	455.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.22	kPa	450.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.99	kPa	445.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.80	kPa	440.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.65	kPa	435.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.53	kPa	430.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.43	kPa	425.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	0.34	kPa	420.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.28	kPa	415.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.22	kPa	410.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.18	kPa	405.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.15	kPa	400.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	3.87	kPa	480.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	3.25	kPa	475.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	2.70	kPa	470.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	2.23	kPa	465.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.84	kPa	460.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.52	kPa	455.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.24	kPa	450.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.00	kPa	445.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.81	kPa	440.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.64	kPa	435.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.53	kPa	430.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.43	kPa	425.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	0.34	kPa	420.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.28	kPa	415.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.22	kPa	410.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.18	kPa	405.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.16	kPa	400.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	3.87	kPa	480.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	3.25	kPa	475.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	2.70	kPa	470.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	2.24	kPa	465.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.85	kPa	460.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.52	kPa	455.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.24	kPa	450.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.01	kPa	445.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.82	kPa	440.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.67	kPa	435.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.54	kPa	430.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.43	kPa	425.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	0.35	kPa	420.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.28	kPa	415.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.23	kPa	410.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.19	kPa	405.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.15	kPa	400.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	3.77	kPa	480.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	3.15	kPa	475.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	2.17	kPa	465.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis

pvap	1.79	kPa	460.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.47	kPa	455.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	1.20	kPa	450.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.98	kPa	445.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.80	kPa	440.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.66	kPa	435.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	0.52	kPa	430.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
pvap	2.62	kPa	470.00	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
sfust	49.90	J/mol×K	373.00	NIST Webbook
sfust	48.20	J/mol×K	373.20	NIST Webbook
sfust	46.20	J/mol×K	371.40	NIST Webbook
sfust	46.10	J/mol×K	371.70	NIST Webbook
ssubt	304.90	J/mol×K	298.15	NIST Webbook

svapt	249.30	J/mol×K	350.00	NIST Webbook
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	485.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49964e+01
Coeff. B	-5.57632e+03
Coeff. C	-7.18810e+01
Temperature range (K), min.	451.00
Temperature range (K), max.	647.66

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.07381e+02
Coeff. B	-1.29131e+04
Coeff. C	-1.29796e+01
Coeff. D	4.34300e-06
Temperature range (K), min.	372.15
Temperature range (K), max.	869.25

Sources

Phase Behavior Data of (CO2 + Toluene + Phenanthrene) and (CO2 + (Methanol + Phenanthrene) Systems at High Pressure: Combined experiments to measure low sublimation pressures and diffusion coefficients of Phenanthrene in Binary Mixtures of C1-C4 Alcohols at 298.2 K:

<https://www.doi.org/10.1021/acs.jced.7b00126>
https://en.wikipedia.org/wiki/Joback_method
<https://www.doi.org/10.1016/j.tca.2006.10.021>
<https://www.doi.org/10.1021/je900599q>

Measurement of the Phase Behavior of the Ternary System Carbon Dioxide + Ethanol + Methanol and Vapor Pressures of Some Deuterated Hydrocarbons: Liquid Vapor Pressure Effects:	https://www.doi.org/10.1021/je0496239
Solubilities of Palmitic Acid + Capsaicin in Supercritical Carbon Dioxide	https://www.doi.org/10.1021/je800091s
Enthalpies of fusion, vaporisation and sublimation of crown ethers	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Masses determined by thermogravimetry and differential scanning calorimetry: Aqueous Solubility Prediction Method:	https://www.doi.org/10.1021/acs.jced.7b00576
Solubility of iodopropynyl butylcarbamate in supercritical carbon dioxide	https://www.doi.org/10.1016/j.tca.2016.03.013
Solubility of Phenanthrene in Binary Mixtures of C1-C4 Alcohols + KDB	http://link.springer.com/article/10.1007/BF02311772
4-P-Propanol and Ethanol + Methanol at 298.15 K: KDB Vapor Pressure Data:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
NIST Webbook:	https://www.doi.org/10.1016/j.fluid.2008.05.010
Thermodynamic study of (anthracene + phenanthrene) solid state mixtures: Estimated Solubility Method:	https://www.doi.org/10.1021/je900027h
Determination of Henry's Law Constant Using Diffusion in Air and Water	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=789
Solubility of Anthracene and Phenanthrene in Ethanol + 2,2,4,4-tetramethylpentane	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=789
Critical point measurement of some polycyclic aromatic hydrocarbons: The design, construction, and testing of a new Knudsen effusion apparatus:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85018&Units=SI
Development and test of a new Knudsen effusion apparatus for the measurement of low vapour pressures: phenanthrene and carbazole in gas phase	https://www.doi.org/10.1016/j.jct.2015.06.021
Gas phase enthalpy of formation of the biphenyls using combustion calorimetry and elimination analysis by thermogravimetry: Analysis of the Group 1 Methods in the case of methyl and phenyl substituted hydantoin:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Elimination of Tar in Biomass Gasification Process: Liquid Liquid Equilibrium of Ternary Systems {Water + Solvent (p-Xylene and Methyl Hexadecanoate) + Model Molecules of Tar (Thiophene, Pyridine, Naphthalene, Phenanthrene, and Anthracene)}:	https://www.doi.org/10.1021/je300954s

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rnpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
ssubt:	Entropy of sublimation at a given temperature
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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