Triphenylene

Other names:	1,2,3,4-DIBENZNAPHTHALENE
	9,10-Benzophenanthrene
	9,10-Benzphenanthrene
	Benzo[l]phenanthrene
	ISOCHRYSENE
Inchi:	InChI=1S/C18H12/c1-2-8-14-13(7-1)15-9-3-4-11-17(15)18-12-6-5-10-16(14)18/h1-12H
InchiKey:	SLGBZMMZGDRARJ-UHFFFAOYSA-N
Formula:	C18H12
SMILES:	c1ccc2c(c1)c1ccccc1c1ccccc21
Mol. weight [g/mol]:	228.29
CAS:	217-59-4

Physical Properties

Property code	Value	Unit	Source
affp	818.00	kJ/mol	NIST Webbook
affp	819.20	kJ/mol	NIST Webbook
basg	791.20	kJ/mol	NIST Webbook
basg	792.90	kJ/mol	NIST Webbook
chs	-8939.24 ± 0.46	kJ/mol	NIST Webbook
chs	-8945.40 ± 2.20	kJ/mol	NIST Webbook
chs	-8950.00 ± 1.20	kJ/mol	NIST Webbook
ea	0.28 ± 0.01	eV	NIST Webbook
ea	0.14	eV	NIST Webbook
gf	513.78	kJ/mol	Joback Method
hf	270.10 ± 4.40	kJ/mol	NIST Webbook
hfs	141.00 ± 0.46	kJ/mol	NIST Webbook
hfs	151.80 ± 1.50	kJ/mol	NIST Webbook
hfs	150.00 ± 2.90	kJ/mol	NIST Webbook
hfus	26.70	kJ/mol	Joback Method
hsub	127.00 ± 4.00	kJ/mol	NIST Webbook
hsub	120.10 ± 3.30	kJ/mol	NIST Webbook
hsub	107.00	kJ/mol	NIST Webbook
hsub	127.00 ± 4.00	kJ/mol	NIST Webbook
hvap	106.10 ± 3.90	kJ/mol	NIST Webbook
ie	8.17	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
ie	8.09	eV	NIST Webbook

ie	8.10	eV	NIST Webbook
ie	8.08	eV	NIST Webbook
ie	7.88 ± 0.02	eV	NIST Webbook
ie	8.20 ± 0.30	eV	NIST Webbook
ie	7.84 ± 0.01	eV	NIST Webbook
ie	7.89 ± 0.04	eV	NIST Webbook
ie	7.84 ± 0.05	eV	NIST Webbook
ie	8.00 ± 0.20	eV	NIST Webbook
ie	7.87 ± 0.02	eV	NIST Webbook
ie	7.88	eV	NIST Webbook
ie	7.86	eV	NIST Webbook
ie	8.13	eV	NIST Webbook
log10ws	-6.74		Aqueous Solubility Prediction Method
log10ws	-6.73		Estimated Solubility Method
logp	5.146		Crippen Method
mcvol	182.340	ml/mol	McGowan Method
pc	2511.00	kPa	KDB
rinpol	2395.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	399.75		NIST Webbook
rinpol	399.60		NIST Webbook
rinpol	399.64		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	399.84		NIST Webbook
rinpol	400.10		NIST Webbook
rinpol	399.98		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	401.45		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	398.78		NIST Webbook
rinpol	397.36		NIST Webbook
rinpol	399.63		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	403.65		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	399.40		NIST Webbook

rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	399.57		NIST Webbook
rinpol	399.71		NIST Webbook
rinpol	399.56		NIST Webbook
rinpol	399.40		NIST Webbook
rinpol	2411.00		NIST Webbook
rinpol	2401.00		NIST Webbook
rinpol	399.94		NIST Webbook
rinpol	2411.00		NIST Webbook
ss	254.68	J/mol×K	NIST Webbook
tb	698.00	K	KDB
tb	711.20	K	NIST Webbook
tc	1013.20	K	KDB
tf	473.60 ± 0.40	K	NIST Webbook
tf	471.40	K	Aqueous Solubility Prediction Method
tf	468.00 ± 3.00	K	NIST Webbook
tf	474.00 ± 3.00	K	NIST Webbook
tf	464.00	K	KDB
tt	471.01 ± 0.01	K	NIST Webbook
vc	0.700	m3/kmol	KDB
zc	0.2086470		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.00	J/mol×K	704.82	Joback Method
cpg	532.31	J/mol×K	924.47	Joback Method
cpg	521.02	J/mol×K	880.54	Joback Method
cpg	509.15	J/mol×K	836.61	Joback Method
cpg	496.51	J/mol×K	792.68	Joback Method
cpg	482.86	J/mol×K	748.75	Joback Method
cpg	543.24	J/mol×K	968.39	Joback Method
cps	259.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0007890	Pa×s	661.05	Joback Method
dvisc	0.0008825	Pa×s	617.27	Joback Method
dvisc	0.0010040	Pa×s	573.50	Joback Method

dvisc	0.0011669	Pa×s	529.73	Joback Method
dvisc	0.0013935	Pa×s	485.95	Joback Method
dvisc	0.0007153	Pa×s	704.82	Joback Method
dvisc	0.0017235	Pa×s	442.18	Joback Method
hfust	24.74	kJ/mol	471.00	NIST Webbook
hfust	24.74	kJ/mol	471.00	NIST Webbook
hfust	23.00	kJ/mol	471.20	NIST Webbook
hfust	24.19	kJ/mol	471.06	NIST Webbook
hfust	24.74	kJ/mol	471.01	NIST Webbook
hsubt	118.00 ± 4.00	kJ/mol	368.00	NIST Webbook
hsubt	110.00	kJ/mol	293.00	NIST Webbook
hsubt	118.00 ± 4.20	kJ/mol	338.00	NIST Webbook
hsubt	107.60	kJ/mol	415.50	NIST Webbook
hsubt	114.50	kJ/mol	383.00	NIST Webbook
hsubt	107.10	kJ/mol	425.00	NIST Webbook
hvapt	88.50	kJ/mol	398.00	NIST Webbook
hvapt	67.70	kJ/mol	651.50	NIST Webbook
psub	3.75e-04	kPa	399.10	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	2.58e-04	kPa	395.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	2.64e-04	kPa	394.90	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.78e-04	kPa	390.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method

psub	4.64e-05	kPa	378.00	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.51e-05	kPa	377.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	4.48e-05	kPa	377.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.70e-05	kPa	368.40	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
psub	1.16e-04	kPa	386.70	Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method
pvap	1.69e-07	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.70e-07	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.39e-06	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.76e-06	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.31e-05	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.36e-05	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.63e-04	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.91e-04	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.85e-04	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.90e-03	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.87e-03	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.52e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.04	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.07	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.30e-07	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.19	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.29	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.44	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.64	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.92	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.12	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

sfust	52.53	J/mol×K	471.01	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-5.59978e+01
Coeff. B	-3.74901e+03
Coeff. C	1.03308e+01
Coeff. D	-4.18271e-06
Temperature range (K), min.	533.15
Temperature range (K), max.	773.15

Sources

Solubility of Solid Polycyclic Aromatic Hydrocarbons in Pressurized Hot Water at Temperatures from 313 K to the Melting Point:	https://www.doi.org/10.1021/je050427r
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C217594&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=806
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/files/research/kdb/mol/mol806.mol
Vapor Pressures and Enthalpies of Sublimation of Ten Polycyclic Aromatic Hydrocarbons Determined via the Knudsen Effusion Method:	https://www.doi.org/10.1021/je7005133

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity

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
hsub:	Enthalpy of sublimation at standard conditions
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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