Phenanthrene, 2-methyl-

Other names: 2-Methylphenanthrene
Inchi: InChI=1S/C15H12/c1-11-6-9-15-13(10-11)8-7-12-4-2-3-5-14(12)15/h2-10H,1H3
InchiKey: KANLOADZXMMCQA-UHFFFAOYSA-N
Formula: C15H12
SMILES: Cc1ccc2c(ccc3ccccc32)c1
Mol. weight [g/mol]: 192.26
CAS: 2531-84-2

Physical Properties

Property code	Value	Unit	Source
gf	381.87	kJ/mol	Joback Method
hf	242.80	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
ie	7.90 ± 0.04	eV	NIST Webbook
log10ws	-5.84		Aqueous Solubility Prediction Method
log10ws	-5.84		Estimated Solubility Method
logp	4.301		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	320.34		NIST Webbook
rinpol	319.03		NIST Webbook
rinpol	319.93		NIST Webbook
rinpol	319.78		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1909.30		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1945.00		NIST Webbook

rinpol	319.78		NIST Webbook
rinpol	312.30		NIST Webbook
rinpol	320.17		NIST Webbook
rinpol	319.50		NIST Webbook
rinpol	319.85		NIST Webbook
rinpol	319.03		NIST Webbook
rinpol	319.76		NIST Webbook
rinpol	320.08		NIST Webbook
rinpol	319.48		NIST Webbook
rinpol	320.39		NIST Webbook
rinpol	320.34		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	320.08		NIST Webbook
rinpol	320.10		NIST Webbook
rinpol	319.76		NIST Webbook
rinpol	319.93		NIST Webbook
rinpol	320.17		NIST Webbook
rinpol	318.50		NIST Webbook
rinpol	319.67		NIST Webbook
rinpol	319.67		NIST Webbook
rinpol	319.76		NIST Webbook
rinpol	319.99		NIST Webbook
rinpol	316.40		NIST Webbook
rinpol	336.17		NIST Webbook
rinpol	319.31		NIST Webbook
rinpol	316.40		NIST Webbook
rinpol	319.50		NIST Webbook
rinpol	320.20		NIST Webbook
rinpol	319.50		NIST Webbook
rinpol	320.97		NIST Webbook
rinpol	319.13		NIST Webbook
rinpol	316.40		NIST Webbook
rinpol	320.17		NIST Webbook
rinpol	320.25		NIST Webbook
rinpol	320.30		NIST Webbook
rinpol	321.28		NIST Webbook
rinpol	318.50		NIST Webbook
rinpol	316.40		NIST Webbook
rinpol	320.20		NIST Webbook
rinpol	319.99		NIST Webbook
rinpol	320.17		NIST Webbook
ripol	2907.00		NIST Webbook
ripol	2907.00		NIST Webbook
tb	617.20	K	Joback Method

tc	866.35	K	Joback Method
tf	329.00 ± 3.00	K	NIST Webbook
tf	330.00 ± 3.00	K	NIST Webbook
tf	328.00 ± 4.00	K	NIST Webbook
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.22	J/mol×K	617.20	Joback Method
cpg	396.50	J/mol×K	658.73	Joback Method
cpg	410.54	J/mol×K	700.25	Joback Method
cpg	423.46	J/mol×K	741.78	Joback Method
cpg	435.41	J/mol×K	783.30	Joback Method
cpg	446.52	J/mol×K	824.83	Joback Method
cpg	456.90	J/mol×K	866.35	Joback Method
dvisc	0.0013574	Pa×s	375.67	Joback Method
dvisc	0.0010334	Pa×s	415.93	Joback Method
dvisc	0.0008255	Pa×s	456.18	Joback Method
dvisc	0.0006839	Pa×s	496.44	Joback Method
dvisc	0.0005828	Pa×s	536.69	Joback Method
dvisc	0.0005079	Pa×s	576.95	Joback Method
dvisc	0.0004506	Pa×s	617.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.70	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37620e+01

Coeff. B	-4.67696e+03
Coeff. C	-1.14900e+02
Temperature range (K), min.	462.00
Temperature range (K), max.	668.35

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2531842&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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