Phenanthrene, 3,6-dimethyl-

Other names: 3,6-Dimethylphenanthrene
Inchi: InChI=1S/C16H14/c1-11-3-5-13-7-8-14-6-4-12(2)10-16(14)15(13)9-11/h3-10H,1-2H3
InchiKey: OMIBPZBOAJFEJS-UHFFFAOYSA-N
Formula: C16H14
SMILES: Cc1ccc2ccc3ccc(C)cc3c2c1
Mol. weight [g/mol]: 206.28
CAS: 1576-67-6

Physical Properties

Property code	Value	Unit	Source
gf	380.66	kJ/mol	Joback Method
hf	210.69	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
ie	7.60 ± 0.03	eV	NIST Webbook
log10ws	-6.03		Crippen Method
logp	4.610		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	337.83		NIST Webbook
rinpol	335.46		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	1999.80		NIST Webbook
rinpol	2008.20		NIST Webbook
rinpol	1979.00		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	336.41		NIST Webbook
rinpol	336.60		NIST Webbook
rinpol	336.46		NIST Webbook
rinpol	337.00		NIST Webbook
rinpol	336.53		NIST Webbook
rinpol	335.40		NIST Webbook
rinpol	337.83		NIST Webbook
rinpol	335.46		NIST Webbook

rinpol	337.80		NIST Webbook
rinpol	340.10		NIST Webbook
rinpol	344.90		NIST Webbook
rinpol	335.40		NIST Webbook
rinpol	336.60		NIST Webbook
rinpol	337.83		NIST Webbook
rinpol	338.65		NIST Webbook
rinpol	338.60		NIST Webbook
rinpol	337.83		NIST Webbook
tb	636.20	K	NIST Webbook
tc	889.67	K	Joback Method
tf	399.46	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.69	J/mol×K	645.06	Joback Method
cpg	497.31	J/mol×K	848.90	Joback Method
cpg	485.63	J/mol×K	808.13	Joback Method
cpg	473.15	J/mol×K	767.36	Joback Method
cpg	459.74	J/mol×K	726.60	Joback Method
cpg	445.30	J/mol×K	685.83	Joback Method
cpg	508.31	J/mol×K	889.67	Joback Method
dvisc	0.0004320	Pa×s	645.06	Joback Method
dvisc	0.0004850	Pa×s	604.13	Joback Method
dvisc	0.0005537	Pa×s	563.19	Joback Method
dvisc	0.0006454	Pa×s	522.26	Joback Method
dvisc	0.0007722	Pa×s	481.33	Joback Method
dvisc	0.0009553	Pa×s	440.39	Joback Method
dvisc	0.0012344	Pa×s	399.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37543e+01

Coeff. B	-4.78678e+03
Coeff. C	-1.19348e+02
Temperature range (K), min.	474.80
Temperature range (K), max.	686.31

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1576676&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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