1,7-DIMETHYLPHENANTHRENE

Other names: 1,7-Dimethylphenanthrene
Pimanthrene
Inchi: InChI=1S/C16H14/c1-11-6-8-15-13(10-11)7-9-14-12(2)4-3-5-16(14)15/h3-10H,1-2H3
InchiKey: NZCMUISOTIPJAM-UHFFFAOYSA-N
Formula: C16H14
SMILES: Cc1ccc2c(ccc3c(C)cccc32)c1
Mol. weight [g/mol]: 206.29

Physical Properties

Property code	Value	Unit	Source
af	0.5129		Cheméo Relay (1.0)
gf	380.66	kJ/mol	Joback Method
hf	146.23	kJ/mol	Cheméo Relay (1.0)
hfus	24.11	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Cheméo Relay (1.0)
ie	7.55	eV	Cheméo Relay (1.0)
log10ws	-6.25		Cheméo Relay (1.0)
logp	4.610		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	341.41		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	342.30		NIST Webbook
rinpol	343.10		NIST Webbook
rinpol	342.60		NIST Webbook
rinpol	343.00		NIST Webbook
rinpol	342.04		NIST Webbook
rinpol	343.52		NIST Webbook
rinpol	341.54		NIST Webbook
rinpol	341.80		NIST Webbook
tb	642.96	K	Cheméo Relay (1.0)
tc	893.31	K	Cheméo Relay (1.0)
tf	365.75	K	Cheméo Relay (1.0)
vc	0.661	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.69	J/mol×K	645.06	Joback Method
cpg	508.31	J/mol×K	889.67	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
dvisc	0.0006454	Pa×s	522.26	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	0.0012344	Pa×s	399.46	Joback Method
dvisc	0.0007722	Pa×s	481.33	Joback Method
dvisc	0.0009553	Pa×s	440.39	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C483874&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume