Phenanthrene, 1,6-dimethyl-

Other names: 1,6-dimethylphenanthrene
Inchi: InChI=1S/C16H14/c1-11-6-7-13-8-9-14-12(2)4-3-5-15(14)16(13)10-11/h3-10H,1-2H3
InchiKey: YQMHHSZADKJARE-UHFFFAOYSA-N
Formula: C16H14
SMILES: Cc1ccc2ccc3c(C)cccc3c2c1
Mol. weight [g/mol]: 206.28
CAS: 20291-74-1

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
log10ws	-6.03		Crippen Method
logp	4.610		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	340.50		NIST Webbook
tb	645.06	K	Joback Method
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	445.30	J/mol×K	685.83	Joback Method
cpg	459.74	J/mol×K	726.60	Joback Method
cpg	473.15	J/mol×K	767.36	Joback Method
cpg	485.63	J/mol×K	808.13	Joback Method
cpg	497.31	J/mol×K	848.90	Joback Method
cpg	508.31	J/mol×K	889.67	Joback Method

dvisc	0.0012344	Pa×s	399.46	Joback Method
dvisc	0.0009553	Pa×s	440.39	Joback Method
dvisc	0.0007722	Pa×s	481.33	Joback Method
dvisc	0.0006454	Pa×s	522.26	Joback Method
dvisc	0.0005537	Pa×s	563.19	Joback Method
dvisc	0.0004850	Pa×s	604.13	Joback Method
dvisc	0.0004320	Pa×s	645.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20291741&Units=SI
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
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