Phenanthrene, 1,6,7-trimethyl-

Other names: 1,6,7-trimethylphenanthrene
Inchi: InChI=1S/C17H16/c1-11-5-4-6-16-15(11)8-7-14-9-12(2)13(3)10-17(14)16/h4-10H,1-3H3
InchiKey: XLZALQPCVKISNV-UHFFFAOYSA-N
Formula: C17H16
SMILES: Cc1cc2ccc3c(C)cccc3c2cc1C
Mol. weight [g/mol]: 220.31
CAS: 20291-77-4

Physical Properties

Property code	Value	Unit	Source
gf	379.45	kJ/mol	Joback Method
hf	178.58	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	4.918		Crippen Method
mcvol	187.710	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	672.92	K	Joback Method
tc	913.19	K	Joback Method
tf	423.25	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.54	J/mol×K	672.92	Joback Method
cpg	549.32	J/mol×K	873.15	Joback Method
cpg	537.11	J/mol×K	833.10	Joback Method
cpg	524.14	J/mol×K	793.06	Joback Method
cpg	510.29	J/mol×K	753.01	Joback Method
cpg	495.46	J/mol×K	712.97	Joback Method
cpg	560.86	J/mol×K	913.19	Joback Method
dvisc	0.0004125	Pa×s	672.92	Joback Method

dvisc	0.0004614	Pa×s	631.31	Joback Method
dvisc	0.0005244	Pa×s	589.70	Joback Method
dvisc	0.0006077	Pa×s	548.09	Joback Method
dvisc	0.0007214	Pa×s	506.47	Joback Method
dvisc	0.0008831	Pa×s	464.86	Joback Method
dvisc	0.0011249	Pa×s	423.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20291774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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