Pyrene, 1,2,3,3a,4,5-hexahydro-

Other names: 1,2,3,3a,4,5-Hexahydropyrene
1,2,3,9,10,10a-Hexahydropyrene
Inchi: InChI=1S/C16H16/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1,3-4,7,9,14H,2
InchiKey: AEFBNJXWRHSZGO-UHFFFAOYSA-N
Formula: C16H16
SMILES: c1cc2c3c4c(ccc3c1)CCCC4CC2
Mol. weight [g/mol]: 208.30
CAS: 5385-37-5

Physical Properties

Property code	Value	Unit	Source
gf	403.22	kJ/mol	Joback Method
hf	185.56	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	57.25	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.206		Crippen Method
mcvol	171.360	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	644.23	K	Joback Method
tc	892.20	K	Joback Method
tf	406.88	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.16	J/mol×K	644.23	Joback Method
cpg	535.12	J/mol×K	850.88	Joback Method
cpg	521.78	J/mol×K	809.55	Joback Method
cpg	507.60	J/mol×K	768.22	Joback Method
cpg	492.39	J/mol×K	726.89	Joback Method
cpg	475.98	J/mol×K	685.56	Joback Method
cpg	547.81	J/mol×K	892.20	Joback Method

dvisc	0.0013641	Pa×s	644.23	Joback Method
dvisc	0.0014521	Pa×s	604.67	Joback Method
dvisc	0.0015592	Pa×s	565.11	Joback Method
dvisc	0.0016923	Pa×s	525.56	Joback Method
dvisc	0.0018615	Pa×s	486.00	Joback Method
dvisc	0.0020824	Pa×s	446.44	Joback Method
dvisc	0.0023809	Pa×s	406.88	Joback Method

Sources

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=C5385375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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