

C35 17A,21B,22S-Hopane

Inchi: InChI=1S/C35H62/c1-24(2)12-10-13-25(3)26-16-21-32(6)27(26)17-22-34(8)29(32)14-15-35
InchiKey: STDQCAQCXFHIQA-MXSLBLIISA-N
Formula: C35H62
SMILES: CC(C)CCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 482.87

Physical Properties

Property code	Value	Unit	Source
gf	404.09	kJ/mol	Joback Method
hf	-474.75	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-11.05		Crippen Method
logp	10.940		Crippen Method
mcvol	449.710	ml/mol	McGowan Method
pc	729.67	kPa	Joback Method
rinsol	3606.00		NIST Webbook
tb	1036.49	K	Joback Method
tc	1277.54	K	Joback Method
tf	621.09	K	Joback Method
vc	1.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1857.54	J/mol×K	1036.49	Joback Method
cpg	1919.10	J/mol×K	1076.67	Joback Method
cpg	1985.81	J/mol×K	1116.84	Joback Method
cpg	2058.46	J/mol×K	1157.02	Joback Method
cpg	2137.87	J/mol×K	1197.19	Joback Method
cpg	2224.83	J/mol×K	1237.37	Joback Method
cpg	2320.15	J/mol×K	1277.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R56361&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	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

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