C32 17A,21B,22S-Hopane

Inchi: InChI=1S/C32H56/c1-9-11-22(2)23-14-19-29(5)24(23)15-20-31(7)26(29)12-13-27-30(6)1
InchiKey: OWRSREGIRFCWIJ-UJRAVCPWSA-N
Formula: C32H56
SMILES: CCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 440.79

Physical Properties

Property code	Value	Unit	Source
gf	381.27	kJ/mol	Joback Method
hf	-407.55	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-10.03		Crippen Method
logp	9.914		Crippen Method
mcvol	407.440	ml/mol	McGowan Method
pc	853.96	kPa	Joback Method
rinpol	3312.00		NIST Webbook
tb	968.29	K	Joback Method
tc	1208.02	K	Joback Method
tf	602.28	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1609.29	J/mol×K	968.29	Joback Method
cpg	1661.06	J/mol×K	1008.24	Joback Method
cpg	1716.75	J/mol×K	1048.20	Joback Method
cpg	1777.14	J/mol×K	1088.15	Joback Method
cpg	1843.00	J/mol×K	1128.11	Joback Method
cpg	1915.12	J/mol×K	1168.06	Joback Method
cpg	1994.27	J/mol×K	1208.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56307&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

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
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