C33-Hopane, 17aH, 21bH, 22S

Inchi: InChI=1S/C33H58/c1-9-10-12-23(2)24-15-20-30(5)25(24)16-21-32(7)27(30)13-14-28-31(
InchiKey: KTWXNNDHFXEEFL-AZENOIHOSA-N
Formula: C33H58
SMILES: CCCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 454.81

Physical Properties

Property code	Value	Unit	Source
gf	389.69	kJ/mol	Joback Method
hf	-428.19	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-10.45		Crippen Method
logp	10.304		Crippen Method
mcvol	421.530	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinpol	3340.00		NIST Webbook
tb	991.17	K	Joback Method
tc	1229.95	K	Joback Method
tf	613.55	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1689.90	J/mol×K	991.17	Joback Method
cpg	1744.45	J/mol×K	1030.97	Joback Method
cpg	1803.28	J/mol×K	1070.76	Joback Method
cpg	1867.15	J/mol×K	1110.56	Joback Method
cpg	1936.84	J/mol×K	1150.35	Joback Method
cpg	2013.12	J/mol×K	1190.15	Joback Method
cpg	2096.77	J/mol×K	1229.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R553674&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
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

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