C34 17A,21B,22S-Hopane

Inchi: InChI=1S/C34H60/c1-9-10-11-13-24(2)25-16-21-31(5)26(25)17-22-33(7)28(31)14-15-29-
InchiKey: BFOUVXJORMEENT-ZXHLYZCYSA-N
Formula: C34H60
SMILES: CCCCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 468.84

Physical Properties

Property code	Value	Unit	Source
gf	398.11	kJ/mol	Joback Method
hf	-448.83	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-10.87		Crippen Method
logp	10.694		Crippen Method
mcvol	435.620	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	3507.00		NIST Webbook
rinpol	3507.00		NIST Webbook
tb	1014.05	K	Joback Method
tc	1252.75	K	Joback Method
tf	624.82	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1772.68	J/mol×K	1014.05	Joback Method
cpg	1830.40	J/mol×K	1053.83	Joback Method
cpg	1892.78	J/mol×K	1093.62	Joback Method
cpg	1960.59	J/mol×K	1133.40	Joback Method
cpg	2034.62	J/mol×K	1173.18	Joback Method
cpg	2115.64	J/mol×K	1212.96	Joback Method
cpg	2204.43	J/mol×K	1252.75	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=R56343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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