C33-25-Norhopane, 17aH, 21bH, 22S

Inchi: InChI=1S/C32H56/c1-8-9-11-22(2)23-15-19-30(5)26(23)17-21-32(7)28(30)14-13-27-24-1
InchiKey: XCRHOWRYNNGKCR-DCDBGDEKSA-N
Formula: C32H56
SMILES: CCCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 440.79

Physical Properties

Property code	Value	Unit	Source
gf	386.76	kJ/mol	Joback Method
hf	-422.79	kJ/mol	Joback Method
hfus	33.35	kJ/mol	Joback Method
hvap	80.89	kJ/mol	Joback Method
log10ws	-10.03		Crippen Method
logp	9.914		Crippen Method
mcvol	407.440	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3301.00		NIST Webbook
rinpol	3301.00		NIST Webbook
tb	968.05	K	Joback Method
tc	1203.22	K	Joback Method
tf	578.38	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.16	J/mol×K	968.05	Joback Method
cpg	1651.50	J/mol×K	1007.24	Joback Method
cpg	1700.46	J/mol×K	1046.44	Joback Method
cpg	1752.67	J/mol×K	1085.63	Joback Method
cpg	1808.76	J/mol×K	1124.83	Joback Method
cpg	1869.35	J/mol×K	1164.02	Joback Method
cpg	1935.08	J/mol×K	1203.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R553654&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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