C32-25-Norhopane, 17aH, 21bH, 22R

Inchi: InChI=1S/C31H54/c1-8-10-21(2)22-14-18-29(5)25(22)16-20-31(7)27(29)13-12-26-23-11-
InchiKey: GYGSPXRBNGXRQD-MVUXDMHWSA-N
Formula: C31H54
SMILES: CCCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 426.76

Physical Properties

Property code	Value	Unit	Source
gf	378.34	kJ/mol	Joback Method
hf	-402.15	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	9.524		Crippen Method
mcvol	393.350	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	3231.00		NIST Webbook
rinpol	3231.00		NIST Webbook
tb	945.17	K	Joback Method
tc	1181.45	K	Joback Method
tf	567.11	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1528.73	J/mol×K	945.17	Joback Method
cpg	1573.14	J/mol×K	984.55	Joback Method
cpg	1619.88	J/mol×K	1023.93	Joback Method
cpg	1669.59	J/mol×K	1063.31	Joback Method
cpg	1722.91	J/mol×K	1102.69	Joback Method
cpg	1780.46	J/mol×K	1142.07	Joback Method
cpg	1842.88	J/mol×K	1181.45	Joback Method

Sources

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=R553590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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