C31-25-Norhopane, 17aH, 21bH, 22S

Inchi: InChI=1S/C30H52/c1-8-20(2)21-13-17-28(5)24(21)15-19-30(7)26(28)12-11-25-22-10-9-1
InchiKey: WQHKTMBFSRNFHE-QZSUUGAZSA-N
Formula: C30H52
SMILES: CCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 412.73

Physical Properties

Property code	Value	Unit	Source
gf	369.92	kJ/mol	Joback Method
hf	-381.51	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	9.134		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	3127.00		NIST Webbook
tb	922.29	K	Joback Method
tc	1160.47	K	Joback Method
tf	555.84	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1453.99	J/mol×K	922.29	Joback Method
cpg	1496.72	J/mol×K	961.99	Joback Method
cpg	1541.52	J/mol×K	1001.68	Joback Method
cpg	1589.04	J/mol×K	1041.38	Joback Method
cpg	1639.92	J/mol×K	1081.08	Joback Method
cpg	1694.79	J/mol×K	1120.78	Joback Method
cpg	1754.32	J/mol×K	1160.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R553550&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