

C30 17B,21A-Hopane (Moretane)

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C30H52/c1-8-10-21-13-18-27(4)22(21)14-19-29(6)24(27)11-12-25-28(5)17-9-1

HRIQCHSYFFRYPR-IPONBDEGSA-N

C30H52

CCCC1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C

412.73

Physical Properties

Property code	Value	Unit	Source
gf	366.87	kJ/mol	Joback Method
hf	-360.99	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	9.278		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
pc	953.78	kPa	Joback Method
rinpol	3164.00		NIST Webbook
tb	922.97	K	Joback Method
tc	1163.76	K	Joback Method
tf	594.74	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1454.08	J/mol×K	922.97	Joback Method
cpg	1500.69	J/mol×K	963.10	Joback Method
cpg	1550.52	J/mol×K	1003.23	Joback Method
cpg	1604.33	J/mol×K	1043.37	Joback Method
cpg	1662.91	J/mol×K	1083.50	Joback Method
cpg	1727.04	J/mol×K	1123.63	Joback Method
cpg	1797.50	J/mol×K	1163.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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