17-«beta»-H-Moretane

Inchi: InChI=1S/C30H52/c1-20(2)21-12-17-27(5)22(21)13-18-29(7)24(27)10-11-25-28(6)16-9-1
InchiKey: ZRLNBWWGLOPJIC-YXRLVBGASA-N
Formula: C30H52
SMILES: CC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 412.73

Physical Properties

Property code	Value	Unit	Source
gf	364.43	kJ/mol	Joback Method
hf	-366.27	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	9.134		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	3178.00		NIST Webbook
tb	922.53	K	Joback Method
tc	1166.60	K	Joback Method
tf	579.74	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1454.25	J/mol×K	922.53	Joback Method
cpg	1501.42	J/mol×K	963.21	Joback Method
cpg	1551.88	J/mol×K	1003.89	Joback Method
cpg	1606.44	J/mol×K	1044.56	Joback Method
cpg	1665.90	J/mol×K	1085.24	Joback Method
cpg	1731.08	J/mol×K	1125.92	Joback Method
cpg	1802.80	J/mol×K	1166.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214458&Units=SI

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