

8-«alpha»H,11-Hexahydrofarnesyldrimane

Inchi: InChI=1S/C30H58/c1-23(2)13-9-14-24(3)15-10-16-25(4)17-11-18-27-26(5)19-20-28-29(6)
InchiKey: LBEZSLQQLLUXBF-DITNHSQCSA-N
Formula: C30H58
SMILES: CC(C)CCCC(C)CCCC(C)CCCC1C(C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 418.78

Physical Properties

Property code	Value	Unit	Source
gf	233.39	kJ/mol	Joback Method
hf	-587.95	kJ/mol	Joback Method
hfus	41.37	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Joback Method
log10ws	-10.24		Crippen Method
logp	10.304		Crippen Method
mcvol	411.840	ml/mol	McGowan Method
pc	721.46	kPa	Joback Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		NIST Webbook
tb	901.51	K	Joback Method
tc	1107.86	K	Joback Method
tf	439.74	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.65	J/mol×K	901.51	Joback Method
cpg	1512.08	J/mol×K	935.90	Joback Method
cpg	1543.16	J/mol×K	970.29	Joback Method
cpg	1574.12	J/mol×K	1004.69	Joback Method
cpg	1605.19	J/mol×K	1039.08	Joback Method
cpg	1636.59	J/mol×K	1073.47	Joback Method
cpg	1668.56	J/mol×K	1107.86	Joback Method

Sources

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=R390646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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