

C30 8,14-Secohopane, # 1

Inchi:	InChI=1S/C30H54/c1-20(2)23-16-19-29(7)24(21(3)10-12-26(23)29)13-14-25-22(4)11-15-
InchiKey:	CJRBLAYOLJYSSI-VFVOVWNMSA-N
Formula:	C30H54
SMILES:	CC(C)C1CCC2(C)C(CCC3C(C)CCC4C(C)(C)CCCC34C)C(C)CCC12
Mol. weight [g/mol]:	414.75

Physical Properties

Property code	Value	Unit	Source
gf	294.85	kJ/mol	Joback Method
hf	-496.05	kJ/mol	Joback Method
hfus	35.30	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	9.380		Crippen Method
mcvol	390.120	ml/mol	McGowan Method
pc	836.28	kPa	Joback Method
rinsol	3008.00		NIST Webbook
tb	914.91	K	Joback Method
tc	1142.85	K	Joback Method
tf	506.24	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.73	J/molxK	914.91	Joback Method
cpg	1513.46	J/molxK	952.90	Joback Method
cpg	1551.67	J/molxK	990.89	Joback Method
cpg	1590.75	J/molxK	1028.88	Joback Method
cpg	1631.14	J/molxK	1066.87	Joback Method
cpg	1673.25	J/molxK	1104.86	Joback Method
cpg	1717.48	J/molxK	1142.85	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=R548662&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
mccvol:	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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