

3-hydroxymegastigman-9-one

Inchi:	InChI=1S/C13H24O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h9,11-12,15H,5-8H2,1-4H
InchiKey:	GZFXCGAUFAQBLT-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	CC(=O)CCC1C(C)CC(O)CC1(C)C
Mol. weight [g/mol]:	212.33

Physical Properties

Property code	Value	Unit	Source
gf	-211.33	kJ/mol	Joback Method
hf	-567.92	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	66.31	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.789		Crippen Method
mvol	190.610	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
ripol	2559.00		NIST Webbook
ripol	2559.00		NIST Webbook
tb	648.67	K	Joback Method
tc	841.98	K	Joback Method
tf	365.58	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.95	J/mol×K	648.67	Joback Method
cpg	567.58	J/mol×K	680.89	Joback Method
cpg	584.40	J/mol×K	713.11	Joback Method
cpg	600.48	J/mol×K	745.33	Joback Method
cpg	615.90	J/mol×K	777.54	Joback Method
cpg	630.72	J/mol×K	809.76	Joback Method
cpg	645.02	J/mol×K	841.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R332942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
ripl:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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