

13-nor-Eremophil-1(10)-en-11-one

Inchi:	InChI=1S/C14H22O/c1-10-5-4-6-13-8-7-12(11(2)15)9-14(10,13)3/h6,10,12H,4-5,7-9H2,1
InchiKey:	XVYRIAXPYGHTSG-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(=O)C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]:	206.32
CAS:	54275-21-7

Physical Properties

Property code	Value	Unit	Source
gf	18.31	kJ/mol	Joback Method
hf	-282.70	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1628.70		NIST Webbook
rinpol	1628.70		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2169.00		NIST Webbook
tb	603.86	K	Joback Method
tc	831.60	K	Joback Method
tf	352.21	K	Joback Method
vc	0.691	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.13	J/molxK	603.86	Joback Method
cpg	518.51	J/molxK	641.82	Joback Method

cpg	538.57	J/mol×K	679.77	Joback Method
cpg	557.47	J/mol×K	717.73	Joback Method
cpg	575.36	J/mol×K	755.68	Joback Method
cpg	592.39	J/mol×K	793.64	Joback Method
cpg	608.73	J/mol×K	831.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54275217&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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