

grasshopper ketone

Inchi:	InChI=1S/C14H22O3/c1-10(15)6-5-7-12-13(2,3)8-11(16)9-14(12,4)17/h5,11,16-17H,6,8-9
InchiKey:	UFTGCZKPHFKGLA-UHFFFAOYSA-N
Formula:	C14H22O3
SMILES:	CC(=O)CC=C=C1C(C)(C)CC(O)CC1(C)O
Mol. weight [g/mol]:	238.32

Physical Properties

Property code	Value	Unit	Source
gf	-163.77	kJ/mol	Joback Method
hf	-466.40	kJ/mol	Joback Method
hfus	25.62	kJ/mol	Joback Method
hvap	85.59	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	1.979		Crippen Method
mcvol	201.970	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
ripol	3165.00		NIST Webbook
ripol	3165.00		NIST Webbook
ripol	3170.00		NIST Webbook
ripol	3170.00		NIST Webbook
tb	778.55	K	Joback Method
tc	980.39	K	Joback Method
tf	482.68	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.66	J/molxK	778.55	Joback Method
cpg	630.78	J/molxK	812.19	Joback Method
cpg	645.82	J/molxK	845.83	Joback Method
cpg	660.93	J/molxK	879.47	Joback Method
cpg	676.27	J/molxK	913.11	Joback Method
cpg	691.97	J/molxK	946.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R332808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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