7,8-Epoxy-«alpha»-ionone

Other names:	1-[3-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-2-oxiranyl]ethanone
	Ethanone, 1-[3-(2,6,6-trimethyl-2-cyclohexen-1-yl)oxiranyl]-
Inchi:	InChI=1S/C13H20O2/c1-8-6-5-7-13(3,4)10(8)12-11(15-12)9(2)14/h6,10-12H,5,7H2,1-4H
InchiKey:	SVKGURRUPLWTIE-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CC(=O)C1OC1C1C(C)=CCCC1(C)C
Mol. weight [g/mol]:	208.30
CAS:	37079-64-4

Physical Properties

Property code	Value	Unit	Source
gf	-71.84	kJ/mol	Joback Method
hf	-408.24	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	55.31	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.725		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	598.99	K	Joback Method
tc	820.78	K	Joback Method
tf	366.79	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.44	J/mol×K	598.99	Joback Method
cpg	497.93	J/mol×K	635.96	Joback Method
cpg	516.27	J/mol×K	672.92	Joback Method
cpg	533.58	J/mol×K	709.89	Joback Method

cpg	550.01	J/mol×K	746.85	Joback Method
cpg	565.69	J/mol×K	783.82	Joback Method
cpg	580.76	J/mol×K	820.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37079644&Units=SI
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

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
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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