3-Oxo-«alpha»-ionone

Inchi: InChI=1S/C13H18O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-7,12H,8H2,1-4H3/b6-5-
InchiKey: MLYOGKJJENFVJN-AATRIKPKSA-N
Formula: C13H18O2
SMILES: CC(=O)C=CC1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 206.28
CAS: 79734-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-81.13	kJ/mol	Joback Method
hf	-349.18	kJ/mol	Joback Method
hfus	18.18	kJ/mol	Joback Method
hvap	55.41	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.693		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	641.95	K	Joback Method
tc	872.71	K	Joback Method
tf	389.66	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.42	J/mol×K	641.95	Joback Method
cpg	489.28	J/mol×K	680.41	Joback Method
cpg	506.22	J/mol×K	718.87	Joback Method
cpg	522.33	J/mol×K	757.33	Joback Method
cpg	537.74	J/mol×K	795.79	Joback Method
cpg	552.56	J/mol×K	834.25	Joback Method

cpg	566.89	J/mol×K	872.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79734433&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

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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