3- hydroxy-«alpha»-ionone

Inchi: InChI=1S/C13H20O2/c1-9-5-8-12(15)13(3,4)11(9)7-6-10(2)14/h5-7,11-12,15H,8H2,1-4H
InchiKey: HEGYTNOVZBKKAI-VOTSOKGWSA-N
Formula: C13H20O2
SMILES: CC(=O)C=CC1C(C)=CCC(O)C1(C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-103.07	kJ/mol	Joback Method
hf	-384.05	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	67.53	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.485		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
ripol	2543.00		NIST Webbook
ripol	2543.00		NIST Webbook
tb	661.64	K	Joback Method
tc	864.63	K	Joback Method
tf	378.02	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.33	J/mol×K	661.64	Joback Method
cpg	518.98	J/mol×K	695.47	Joback Method
cpg	533.89	J/mol×K	729.30	Joback Method
cpg	548.16	J/mol×K	763.13	Joback Method
cpg	561.90	J/mol×K	796.96	Joback Method
cpg	575.19	J/mol×K	830.80	Joback Method
cpg	588.14	J/mol×K	864.63	Joback Method

Sources

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=R318184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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