2-Hydroxy-«beta»-Ionone

Other names: 4-(5-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
Inchi: InChI=1S/C13H20O2/c1-9-5-8-12(15)13(3,4)11(9)7-6-10(2)14/h6-7,12,15H,5,8H2,1-4H3/
InchiKey: LXYKLYXWNYMBKQ-VOTSOKGWSA-N
Formula: C13H20O2
SMILES: CC(=O)C=CC1=C(C)CCC(O)C1(C)C
Mol. weight [g/mol]: 208.30
CAS: 67504-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-104.99	kJ/mol	Joback Method
hf	-375.18	kJ/mol	Joback Method
hfus	22.37	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
ripol	2665.00		NIST Webbook
ripol	2665.00		NIST Webbook
tb	671.29	K	Joback Method
tc	875.23	K	Joback Method
tf	394.78	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.33	J/mol×K	671.29	Joback Method
cpg	515.41	J/mol×K	705.28	Joback Method
cpg	529.82	J/mol×K	739.27	Joback Method
cpg	543.66	J/mol×K	773.26	Joback Method
cpg	557.02	J/mol×K	807.25	Joback Method
cpg	570.02	J/mol×K	841.24	Joback Method

cpg	582.75	J/mol×K	875.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67504501&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume