4-Hydroxy-7,8-dihydro-«beta»-ionone

Inchi: InChI=1S/C13H22O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h11,15H,5-8H2,1-4H3
InchiKey: KFZDTDKRRFEMEK-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CC(=O)CCC1=C(C)CC(O)CC1(C)C
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-185.21	kJ/mol	Joback Method
hf	-492.40	kJ/mol	Joback Method
hfus	22.16	kJ/mol	Joback Method
hvap	68.54	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.853		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1373.00		NIST Webbook
rinpol	1373.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1698.00		NIST Webbook
tb	667.13	K	Joback Method
tc	863.93	K	Joback Method
tf	399.86	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.49	J/mol×K	667.13	Joback Method
cpg	538.07	J/mol×K	699.93	Joback Method
cpg	552.96	J/mol×K	732.73	Joback Method
cpg	567.27	J/mol×K	765.53	Joback Method
cpg	581.06	J/mol×K	798.33	Joback Method
cpg	594.42	J/mol×K	831.13	Joback Method

cpg	607.43	J/mol×K	863.93	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=R631155&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume