4-(4-Hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]he

Other names: 3-hydroxy-5,6-epoxy-7,8-dihydro-«beta»-ionone
Inchi: InChI=1S/C13H22O3/c1-9(14)5-6-13-11(2,3)7-10(15)8-12(13,4)16-13/h10,15H,5-8H2,1-4
InchiKey: MGKOACLXSRRQGD-UHFFFAOYSA-N
Formula: C13H22O3
SMILES: CC(=O)CCC12OC1(C)CC(O)CC2(C)C
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-215.77	kJ/mol	Joback Method
hf	-563.98	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	68.39	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.064		Crippen Method
mcvol	185.620	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
ripol	2663.00		NIST Webbook
tb	678.97	K	Joback Method
tc	884.42	K	Joback Method
tf	469.17	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.76	J/mol×K	678.97	Joback Method
cpg	569.16	J/mol×K	713.21	Joback Method
cpg	584.29	J/mol×K	747.45	Joback Method
cpg	599.41	J/mol×K	781.70	Joback Method
cpg	614.81	J/mol×K	815.94	Joback Method
cpg	630.75	J/mol×K	850.18	Joback Method
cpg	647.51	J/mol×K	884.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U190341&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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