2,2,6-Trimethyl-1-(3-methylbuta-1,3-dienyl)-7-oxab

Other names: 3-Hydroxy-5,6-epoxy-«beta»-ionone
Inchi: InChI=1S/C14H22O2/c1-10(2)6-9-14-12(3,4)11(15)7-8-13(14,5)16-14/h6,9,11,15H,1,7-8H
InchiKey: ISUAUJDTROMBDT-RMKNXTFCSA-N
Formula: C14H22O2
SMILES: C=C(C)C=CC12OC1(C)CCC(O)C2(C)C
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	81.08	kJ/mol	Joback Method
hf	-239.18	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.827		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	648.70	K	Joback Method
tc	859.20	K	Joback Method
tf	409.71	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.55	J/mol×K	648.70	Joback Method
cpg	557.70	J/mol×K	683.78	Joback Method
cpg	573.31	J/mol×K	718.87	Joback Method
cpg	588.68	J/mol×K	753.95	Joback Method
cpg	604.15	J/mol×K	789.03	Joback Method
cpg	620.03	J/mol×K	824.12	Joback Method
cpg	636.63	J/mol×K	859.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U191854&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