«beta»-Ionone, 5,6-epoxy

Other names: Â«alphaÂ»-Ionone epoxide (Isomer 1)
Â«alphaÂ»-Ionone epoxide (Isomer 2)
«alpha»-Ionone epoxide (Isomer 1)
«alpha»-Ionone epoxide (Isomer 2)
Inchi: InChI=1S/C13H20O2/c1-9(14)5-6-10-12(2,3)8-7-11-13(10,4)15-11/h5-6,10-11H,7-8H2,1-
InchiKey: ODMUHAHUBCUABS-AATRIKPKSA-N
Formula: C13H20O2
SMILES: CC(=O)C=CC1C(C)(C)CCC2OC21C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	6.76	kJ/mol	Joback Method
hf	-309.77	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	52.82	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.725		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1488.00		NIST Webbook
ripol	2133.00		NIST Webbook
tb	590.71	K	Joback Method
tc	812.55	K	Joback Method
tf	379.37	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.18	J/mol×K	590.71	Joback Method
cpg	492.47	J/mol×K	627.68	Joback Method
cpg	509.60	J/mol×K	664.66	Joback Method
cpg	525.85	J/mol×K	701.63	Joback Method

cpg	541.47	J/mol×K	738.60	Joback Method
cpg	556.73	J/mol×K	775.57	Joback Method
cpg	571.91	J/mol×K	812.55	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=R344039&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