Cyclocitral, 2,3-epoxy

Inchi: InChI=1S/C10H16O2/c1-8(2)5-4-6-9(3)10(8,7-11)12-9/h7H,4-6H2,1-3H3
InchiKey: GQFVNWGJQXEELI-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC1(C)CCCC2(C)OC12C=O
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-67.10	kJ/mol	Joback Method
hf	-302.49	kJ/mol	Joback Method
hfus	8.27	kJ/mol	Joback Method
hvap	45.32	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.923		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
tb	517.61	K	Joback Method
tc	745.43	K	Joback Method
tf	370.85	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.00	J/mol×K	517.61	Joback Method
cpg	363.35	J/mol×K	555.58	Joback Method
cpg	378.11	J/mol×K	593.55	Joback Method
cpg	391.66	J/mol×K	631.52	Joback Method
cpg	404.37	J/mol×K	669.49	Joback Method
cpg	416.61	J/mol×K	707.46	Joback Method
cpg	428.75	J/mol×K	745.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410572&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume