5,5-epoxymethano-2,2,6-trimethyl-7-oxa-bicyclo[4

Inchi: InChI=1S/C14H20O3/c1-12(2)6-7-14(9-16-14)13(3)5-4-10(12)8-11(15)17-13/h8H,4-7,9H
InchiKey: AEHGIVBQTMMUBU-UHFFFAOYSA-N
Formula: C14H20O3
SMILES: CC1(C)CCC2(CO2)C2(C)CCC1=CC(=O)O2
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	-90.12	kJ/mol	Joback Method
hf	-448.20	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	57.95	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.598		Crippen Method
mcvol	184.550	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
ripol	2604.00		NIST Webbook
ripol	2604.00		NIST Webbook
tb	683.60	K	Joback Method
tc	946.16	K	Joback Method
tf	493.62	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.48	J/mol×K	683.60	Joback Method
cpg	573.16	J/mol×K	727.36	Joback Method
cpg	593.41	J/mol×K	771.12	Joback Method
cpg	613.79	J/mol×K	814.88	Joback Method
cpg	634.82	J/mol×K	858.64	Joback Method
cpg	657.07	J/mol×K	902.40	Joback Method

cpg	681.05	J/mol×K	946.16	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=R434914&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