(Z)-6,7-Epoxy-2,6-dimethylnon-8-en-4-one

Inchi: InChI=1S/C11H18O2/c1-5-10-11(4,13-10)7-9(12)6-8(2)3/h5,8,10H,1,6-7H2,2-4H3/t10-,11
InchiKey: WFDCBVPENVGENI-WDEREUQCSA-N
Formula: C11H18O2
SMILES: C=CC1OC1(C)CC(=O)CC(C)C
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-40.35	kJ/mol	Joback Method
hf	-327.10	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	48.73	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.335		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1210.00		NIST Webbook
tb	530.45	K	Joback Method
tc	728.40	K	Joback Method
tf	311.07	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.62	J/mol×K	530.45	Joback Method
cpg	404.25	J/mol×K	563.44	Joback Method
cpg	418.92	J/mol×K	596.43	Joback Method
cpg	432.74	J/mol×K	629.42	Joback Method
cpg	445.81	J/mol×K	662.42	Joback Method
cpg	458.24	J/mol×K	695.41	Joback Method
cpg	470.12	J/mol×K	728.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232114&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