Phellandrene epoxide

Inchi: InChI=1S/C10H16O/c1-8(2)9-3-5-10(6-4-9)7-11-10/h3,5,8-9H,4,6-7H2,1-2H3
InchiKey: LOYQVLUNFXGKGF-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(C)C1C=CC2(CC1)CO2
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	66.53	kJ/mol	Joback Method
hf	-180.71	kJ/mol	Joback Method
hfus	13.11	kJ/mol	Joback Method
hvap	41.29	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.378		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1190.00		NIST Webbook
tb	476.13	K	Joback Method
tc	696.75	K	Joback Method
tf	267.53	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.99	J/mol×K	476.13	Joback Method
cpg	323.72	J/mol×K	512.90	Joback Method
cpg	340.97	J/mol×K	549.67	Joback Method
cpg	356.91	J/mol×K	586.44	Joback Method
cpg	371.69	J/mol×K	623.21	Joback Method
cpg	385.47	J/mol×K	659.98	Joback Method
cpg	398.42	J/mol×K	696.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203691&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