Myrcene epoxide

Other names: Epoxymyrcene
Inchi: InChI=1S/C10H16O/c1-5-8(2)6-7-9-10(3,4)11-9/h5,9H,1-2,6-7H2,3-4H3
InchiKey: DQGZGGZXMOFHLB-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=CC(=C)CCC1OC1(C)C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	161.88	kJ/mol	Joback Method
hf	-72.96	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	39.56	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.686		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1099.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1398.00		NIST Webbook
tb	450.70	K	Joback Method
tc	644.70	K	Joback Method
tf	249.15	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.19	J/mol×K	450.70	Joback Method
cpg	316.98	J/mol×K	483.03	Joback Method
cpg	331.68	J/mol×K	515.37	Joback Method
cpg	345.40	J/mol×K	547.70	Joback Method
cpg	358.23	J/mol×K	580.03	Joback Method
cpg	370.29	J/mol×K	612.36	Joback Method
cpg	381.66	J/mol×K	644.70	Joback Method

Sources

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=R195436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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