4,5-Epoxyterpinolene

Inchi: InChI=1S/C10H16O/c1-7(2)8-4-5-10(3)9(6-8)11-10/h9H,4-6H2,1-3H3
InchiKey: UFPFCBUOSFFMKS-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(C)=C1CCC2(C)OC2C1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	88.02	kJ/mol	Joback Method
hf	-160.81	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	42.08	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.664		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
ripol	1476.00		NIST Webbook
tb	479.66	K	Joback Method
tc	696.53	K	Joback Method
tf	281.69	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.75	J/mol×K	479.66	Joback Method
cpg	323.20	J/mol×K	515.81	Joback Method
cpg	339.28	J/mol×K	551.95	Joback Method
cpg	354.15	J/mol×K	588.10	Joback Method
cpg	367.97	J/mol×K	624.24	Joback Method
cpg	380.91	J/mol×K	660.39	Joback Method
cpg	393.12	J/mol×K	696.53	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=R234294&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume