Isomyrcenone

Inchi: InChI=1S/C10H14O/c1-5-9(4)10(11)7-6-8(2)3/h5-6H,1,4,7H2,2-3H3
InchiKey: VOZLDFIRYMGFSU-UHFFFAOYSA-N
Formula: C10H14O
SMILES: C=CC(=C)C(=O)CC=C(C)C
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	143.20	kJ/mol	Joback Method
hf	-13.81	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	43.38	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.654		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
tb	479.35	K	Joback Method
tc	674.39	K	Joback Method
tf	215.87	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.99	J/mol×K	479.35	Joback Method
cpg	303.37	J/mol×K	511.86	Joback Method
cpg	316.00	J/mol×K	544.36	Joback Method
cpg	327.93	J/mol×K	576.87	Joback Method
cpg	339.19	J/mol×K	609.38	Joback Method
cpg	349.82	J/mol×K	641.88	Joback Method
cpg	359.86	J/mol×K	674.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R517712&Units=SI

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