(Z)-Ocimenol

Inchi: InChI=1S/C10H18O/c1-5-9(2)7-6-8-10(3,4)11/h5,7,11H,1,6,8H2,2-4H3/b9-7-
InchiKey: IJFKZRMIRAVXRK-CLFYSBASSA-N
Formula: C10H18O
SMILES: C=CC(C)=CCCC(C)(C)O
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	58.85	kJ/mol	Joback Method
hf	-177.85	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	52.61	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.670		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
ripol	1662.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	517.87	K	Joback Method
tc	697.57	K	Joback Method
tf	244.90	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.03	J/mol×K	517.87	Joback Method
cpg	360.38	J/mol×K	547.82	Joback Method
cpg	372.99	J/mol×K	577.77	Joback Method
cpg	384.91	J/mol×K	607.72	Joback Method
cpg	396.18	J/mol×K	637.67	Joback Method
cpg	406.83	J/mol×K	667.62	Joback Method
cpg	416.91	J/mol×K	697.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308251&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume