trans-Ocimenol

Inchi: InChI=1S/C10H16O/c1-5-9(4)7-10(11)6-8(2)3/h5-7,10-11H,1H2,2-4H3/b9-7+
InchiKey: DUCHBDMNWUYHGL-VQHVLOKHSA-N
Formula: C10H16O
SMILES: C=CC(C)=CC(O)C=C(C)C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	125.24	kJ/mol	Joback Method
hf	-66.95	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.446		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
ripol	1685.00		NIST Webbook
tb	524.70	K	Joback Method
tc	708.61	K	Joback Method
tf	208.44	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.95	J/mol×K	524.70	Joback Method
cpg	338.47	J/mol×K	555.35	Joback Method
cpg	350.31	J/mol×K	586.00	Joback Method
cpg	361.52	J/mol×K	616.65	Joback Method
cpg	372.13	J/mol×K	647.31	Joback Method
cpg	382.18	J/mol×K	677.96	Joback Method
cpg	391.71	J/mol×K	708.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R295026&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
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