

trans-isopiperitenol

Other names:	trans-p-mentha-1,8-dien-3-ol
Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h6,9-11H,1,4-5H2,2-3H3/t9-,10+/m0/s1
InchiKey:	OLAKPNFIICOONC-VHSXEESVSA-N
Formula:	C10H16O
SMILES:	<chem>C=C(C)C1CCC(C)=CC1O</chem>
Mol. weight [g/mol]:	152.23
CAS:	74410-00-7

Physical Properties

Property code	Value	Unit	Source
gf	12.86	kJ/mol	Joback Method
hf	-206.03	kJ/mol	Joback Method
hfus	16.89	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.280		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1210.20		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1750.00		NIST Webbook
tb	535.96	K	Joback Method
tc	731.65	K	Joback Method
tf	263.98	K	Joback Method
vc	0.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.99	J/mol×K	535.96	Joback Method
cpg	347.03	J/mol×K	568.58	Joback Method

cpg	361.30	J/mol×K	601.19	Joback Method
cpg	374.84	J/mol×K	633.81	Joback Method
cpg	387.67	J/mol×K	666.42	Joback Method
cpg	399.80	J/mol×K	699.04	Joback Method
cpg	411.26	J/mol×K	731.65	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=C74410007&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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