

5-Hydroxyneoisomenthol, trans

Other names:	trans-5-Hydroxyneoisomenthol
Inchi:	InChI=1S/C10H20O2/c1-6(2)10-8(11)4-7(3)5-9(10)12/h6-12H,4-5H2,1-3H3/t7-,8-,9-,10-/
InchiKey:	BUHKNALVIKKDKZ-AATLWQCWSA-N
Formula:	C10H20O2
SMILES:	CC1CC(O)C(C(C)C)C(O)C1
Mol. weight [g/mol]:	172.26

Physical Properties

Property code	Value	Unit	Source
gf	-241.44	kJ/mol	Joback Method
hf	-566.17	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	70.33	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.410		Crippen Method
mcvol	152.640	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1402.00		NIST Webbook
tb	617.66	K	Joback Method
tc	797.97	K	Joback Method
tf	303.76	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.89	J/mol×K	617.66	Joback Method
cpg	506.10	J/mol×K	767.92	Joback Method
cpg	493.86	J/mol×K	737.87	Joback Method
cpg	480.93	J/mol×K	707.81	Joback Method
cpg	467.30	J/mol×K	677.76	Joback Method
cpg	452.95	J/mol×K	647.71	Joback Method
cpg	517.65	J/mol×K	797.97	Joback Method
dvisc	0.0000421	Pa×s	617.66	Joback Method

dvisc	0.0000780	Pa×s	565.34	Joback Method
dvisc	0.0001637	Pa×s	513.03	Joback Method
dvisc	0.0004067	Pa×s	460.71	Joback Method
dvisc	0.0012754	Pa×s	408.39	Joback Method
dvisc	0.0055954	Pa×s	356.08	Joback Method
dvisc	0.0408544	Pa×s	303.76	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=R96301&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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