

2-Hydroxyneoisomenthol, trans

Other names:	trans-2-Hydroxyneoisomenthol
Inchi:	InChI=1S/C10H20O2/c1-6(2)8-5-4-7(3)9(11)10(8)12/h6-12H,4-5H2,1-3H3/t7-,8-,9+,10+/r
InchiKey:	WQFGPARDTSBVLU-AXTSPUMRSA-N
Formula:	C10H20O2
SMILES:	CC(C)C1CCC(C)C(O)C1O
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
mvol	152.640	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	617.66	K	Joback Method
tc	797.97	K	Joback Method
tf	303.76	K	Joback Method
vc	0.557	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0408544	Paxs	303.76	Joback Method
dvisc	0.0055954	Paxs	356.08	Joback Method
dvisc	0.0012754	Paxs	408.39	Joback Method
dvisc	0.0004067	Paxs	460.71	Joback Method
dvisc	0.0001637	Paxs	513.03	Joback Method
dvisc	0.0000780	Paxs	565.34	Joback Method
dvisc	0.0000421	Paxs	617.66	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=R96262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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