Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1«alpha»,2«alpha»,5«beta»)-

Other names: p-Menth-8-en-2-ol, cis-1,2,trans-1,4-
Neodihydrocarveol
5-Isopropenyl-2-methylcyclohexanol, (1«alpha»,2«alpha»,5«beta»)-
Dihydro carveol neo
(1R,2S,5S)-neodihydrocarveol
Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1R,2S,5S)-rel-
Neocarveol, dihydro-
neo-iso-Dihydrocarveol

Inchi: InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)10(11)6-9/h8-11H,1,4-6H2,2-3H3

InchiKey: KRCZYMFUWVJCLI-UHFFFAOYSA-N

Formula: C10H18O

SMILES: C=C(C)C1CCC(C)C(O)C1

Mol. weight [g/mol]: 154.25

CAS: 18675-33-7

Physical Properties

Property code	Value	Unit	Source
gf	-15.18	kJ/mol	Joback Method
hf	-272.68	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.360		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1189.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1189.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1735.00		NIST Webbook

ripol	1783.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1777.00		NIST Webbook
tb	527.15	K	Joback Method
tc	719.80	K	Joback Method
tf	246.46	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.71	J/mol×K	527.15	Joback Method
cpg	367.51	J/mol×K	559.26	Joback Method
cpg	383.50	J/mol×K	591.37	Joback Method
cpg	398.69	J/mol×K	623.47	Joback Method
cpg	413.11	J/mol×K	655.58	Joback Method
cpg	426.76	J/mol×K	687.69	Joback Method
cpg	439.67	J/mol×K	719.80	Joback Method

Sources

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=C18675337&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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