

1,2-Cyclohexanediol, 4-methyl-1-(1-methylethyl)-, (1«alpha»,2«alpha»,4«alpha»)-

Other names: 1-Isopropyl-4-methyl-1,2-cyclohexanediol (1«alpha»,2«alpha»,4«alpha»)-4-Hydroxyneoisomenthol

Inchi:	InChI=1S/C10H20O2/c1-7(2)10(12)5-4-8(3)6-9(10)11/h7-9,11-12H,4-6H2,1-3H3
InchiKey:	OOJJEXXELQNXDL-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CC1CCC(O)(C(C)C)C(O)C1
Mol. weight [g/mol]:	172.26
CAS:	42962-98-1

Physical Properties

Property code	Value	Unit	Source
gf	-239.22	kJ/mol	Joback Method
hf	-530.59	kJ/mol	Joback Method
hfus	13.99	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.554		Crippen Method
mvol	152.640	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1395.00		NIST Webbook
tb	622.57	K	Joback Method
tc	808.83	K	Joback Method
tf	331.90	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.50	J/molxK	622.57	Joback Method
cpg	447.89	J/molxK	653.61	Joback Method
cpg	461.61	J/molxK	684.66	Joback Method
cpg	474.74	J/molxK	715.70	Joback Method
cpg	487.33	J/molxK	746.74	Joback Method
cpg	499.46	J/molxK	777.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C42962981&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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