

2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, trans-

Other names:	(1R,6R)-6-Isopropyl-3-methylcyclohex-2-enol, rel-p-Menth-1-en-3-ol, trans-trans-p-Menth-1-en-3-ol trans-Piperitol 6-Isopropyl-3-methyl-2-cyclohexen-1-ol, (E)-E-Piperitol trans-3-methyl-6-(1-methylethyl)-2-cyclohexen-1-ol 2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, (1R,6R)-rel-Piperitol, trans-trans-Pipertiol (=trans-p-Menth-1-en-3-ol) (E)-Piperitol acetate trans-Piperitol (trans-p-menth-1-en-3-ol) trans-piperitol (= trans- pmenth-1-en-3-ol) trans-6-(isopropyl)-3-methylcyclohex-2-en-1-ol
Inchi:	InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h6-7,9-11H,4-5H2,1-3H3/t9-,10+/m0/s1
InchiKey:	HPOHAUWWDDPHRS-VHSXEESVSA-N
Formula:	C10H18O
SMILES:	CC1=CC(O)C(C(C)C)CC1
Mol. weight [g/mol]:	154.25
CAS:	16721-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-68.87	kJ/mol	Joback Method
hf	-326.95	kJ/mol	Joback Method
hfus	15.96	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.360		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1205.00		NIST Webbook
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ripol	1689.00		NIST Webbook
ripol	1689.00		NIST Webbook
tb	538.96	K	Joback Method
tc	731.46	K	Joback Method
tf	264.70	K	Joback Method
vc	0.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	351.74	J/molxK	538.96	Joback Method
cpg	367.50	J/molxK	571.04	Joback Method
cpg	382.50	J/molxK	603.13	Joback Method
cpg	396.76	J/molxK	635.21	Joback Method
cpg	410.31	J/molxK	667.29	Joback Method
cpg	423.14	J/molxK	699.37	Joback Method
cpg	435.28	J/molxK	731.46	Joback Method
dvisc	0.0240696	Paxs	264.70	Joback Method
dvisc	0.0052446	Paxs	310.41	Joback Method
dvisc	0.0016898	Paxs	356.12	Joback Method
dvisc	0.0007045	Paxs	401.83	Joback Method
dvisc	0.0003512	Paxs	447.54	Joback Method
dvisc	0.0001992	Paxs	493.25	Joback Method
dvisc	0.0001244	Paxs	538.96	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=C16721394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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

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