

trans-(±)-5-hydroxy-«alpha»,«alpha»,4-trimethylcyclohex-3-ene-1-methanol

Other names:	3-Cyclohexene-1-methanol, 5-hydroxy-«alpha»,«alpha»,4-trimethyl-, trans-(.+)-
Inchi:	InChI=1S/C10H18O2/c1-7-4-5-8(6-9(7)11)10(2,3)12/h4,8-9,11-12H,5-6H2,1-3H3
InchiKey:	OMDMTHRBGUBUCO-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC1=CCC(C(C)(C)[O])CC1[O]
Mol. weight [g/mol]:	170.25
CAS:	32226-54-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.52		Crippen Method
logp	2.351		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
tb	543.70	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32226543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/37-522-1/trans-5-hydroxy-alpha-alpha-4-trimethylcyclohex-3-ene-1-methanol.pdf>

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