

5,5,8,8-Tetramethylcyclodecyne

Inchi:	InChI=1S/C14H24/c1-13(2)9-7-5-6-8-10-14(3,4)12-11-13/h7-12H2,1-4H3
InchiKey:	AULNNULHCDQISI-UHFFFAOYSA-N
Formula:	C14H24
SMILES:	CC1(C)CCC#CCCC(C)(C)CC1
Mol. weight [g/mol]:	192.34
CAS:	2198-28-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	4.396		Crippen Method
mcvol	188.660	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2198289&Units=SI

Legend

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

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<https://www.chemeo.com/cid/40-834-1/5-5-8-8-Tetramethylcyclodecyne.pdf>

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