Cyclooctyne,3,3,8,8-tetramethyl-

Inchi: InChI=1S/C12H20/c1-11(2)7-5-6-8-12(3,4)10-9-11/h5-8H2,1-4H3
InchiKey: WVECPOSSBHZOOS-UHFFFAOYSA-N
Formula: C12H20
SMILES: CC1(C)C#CC(C)(C)CCCC1
Mol. weight [g/mol]: 164.29
CAS: 53561-46-9

Physical Properties

Property code	Value	Unit	Source
ie	8.90	eV	NIST Webbook
log10ws	-4.05		Crippen Method
logp	3.616		Crippen Method
mcvol	160.480	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C53561469&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.