1,1,4,4-Tetramethylcyclododec-8-yne

Inchi: InChI=1S/C16H28/c1-15(2)11-9-7-5-6-8-10-12-16(3,4)14-13-15/h7-14H2,1-4H3
InchiKey: JWMCSWXRLWAYIJ-UHFFFAOYSA-N
Formula: C16H28
SMILES: CC1(C)CCCC#CCCCC(C)(C)CC1
Mol. weight [g/mol]: 220.39
CAS: 15753-76-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.73		Crippen Method
logp	5.177		Crippen Method
mcvol	216.840	ml/mol	McGowan Method

Sources

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=C15753761&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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