

Cyclododecyne

Inchi:	InChI=1S/C12H20/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-10H2
InchiKey:	BYDOJAHKOHCCERE-UHFFFAOYSA-N
Formula:	C12H20
SMILES:	C1#CCCCCCCCCCC1
Mol. weight [g/mol]:	164.29
CAS:	1129-90-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	3.904		Crippen Method
mcvol	160.480	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=C1129904&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

Latest version available from:

<https://www.chemeo.com/cid/20-140-3/Cyclododecyne.pdf>

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