

Cycloundecyne

Inchi: InChI=1S/C11H18/c1-2-4-6-8-10-11-9-7-5-3-1/h1-9H2
InchiKey: PJIYBBSKJDMKBC-UHFFFAOYSA-N
Formula: C11H18
SMILES: C1#CCCCCCCCC1
Mol. weight [g/mol]: 150.26
CAS: 702-32-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	3.514		Crippen Method
mcvol	146.390	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=C702329&Units=SI>

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/69-900-6/Cycloundecyne.pdf>

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