

CD

Inchi: InChI=1S/CH/h1H/i1D
InchiKey: VRLIPUYDFBXWCH-MICDWDOJSA-N
Formula: CD
SMILES: [CH]
Mol. weight [g/mol]: 14.02
CAS: 13776-70-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.25		Crippen Method
logp	0.204		Crippen Method
mcvol	18.500	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=C13776700&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/37-005-5/CD.pdf>

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