

2,5-di-(Hydroxymethyl)furan

Inchi: InChI=1S/C6H8O3/c7-3-5-1-2-6(4-8)9-5/h1-2,7-8H,3-4H2
InchiKey: DSLRVRBSNLHVBH-UHFFFAOYSA-N
Formula: C6H8O3
SMILES: OCC1CCC(CO)O1
Mol. weight [g/mol]: 128.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	0.264		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
rinpol	1229.00		NIST Webbook
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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=R614898&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/81-051-5/2-5-di-Hydroxymethyl-furan.pdf>

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