

3-methyl-2-vinylfuran

Inchi: InChI=1S/C7H8O/c1-3-7-6(2)4-5-8-7/h3-5H,1H2,2H3
InchiKey: WAVMEWSWFALXSL-UHFFFAOYSA-N
Formula: C7H8O
SMILES: C=Cc1occc1C
Mol. weight [g/mol]: 108.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	2.231		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
ripol	1183.00		NIST Webbook
ripol	1161.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1161.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R316440&Units=SI>

Legend

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

ripol: Polar retention indices

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