

Furfurol, 5-ethoxymethyl

Inchi: InChI=1S/C8H12O3/c1-2-10-6-8-4-3-7(5-9)11-8/h3-4,9H,2,5-6H2,1H3
InchiKey: PWKAMVGLPNBYPI-UHFFFAOYSA-N
Formula: C8H12O3
SMILES: CCOCc1ccc(CO)o1
Mol. weight [g/mol]: 156.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	1.308		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
ripol	1929.00		NIST Webbook
ripol	1929.00		NIST Webbook

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=R410661&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
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/81-371-0/Furfurol-5-ethoxymethyl.pdf>

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