4(3)-methyl-2-furanmethanol

Other names: 4(3)-methyl-2-furfuryl alcohol
Inchi: InChI=1S/C6H8O2/c1-5-2-6(3-7)8-4-5/h2,4,7H,3H2,1H3
InchiKey: GFZPVRIBUPUXRP-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: Cc1coc(CO)c1
Mol. weight [g/mol]: 112.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.82		Crippen Method
logp	1.080		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1597.00		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=R296905&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