

2-Thiophenemethanol, «alpha»-methyl-

Other names: «alpha»-methylthiophene-2-methanol
Inchi: InChI=1S/C6H8OS/c1-5(7)6-3-2-4-8-6/h2-5,7H,1H3
InchiKey: WUNFIVTVJXZDDJ-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CC(O)c1cccs1
Mol. weight [g/mol]: 128.19
CAS: 2309-47-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.801		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
rinsol	1054.00		NIST Webbook
rinsol	1054.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2309479&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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