

2-propylsulfanylmethyl-furan

Inchi: InChI=1S/C8H12OS/c1-2-6-10-7-8-4-3-5-9-8/h3-5H,2,6-7H2,1H3
InchiKey: WHMYNJRKOCMTCL-UHFFFAOYSA-N
Formula: C8H12OS
SMILES: CCCSCc1ccco1
Mol. weight [g/mol]: 156.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	2.923		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
rinpola	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=R259342&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/13-857-6/2-propylsulfanylmethyl-furan.pdf>

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