Furan, 3-(ethylthio)-2-methyl

Other names: 3-(Ethylthio)-2-methylfuran
Inchi: InChI=1S/C7H10OS/c1-3-9-7-4-5-8-6(7)2/h4-5H,3H2,1-2H3
InchiKey: PHCQIWHGOFNKSP-UHFFFAOYSA-N
Formula: C7H10OS
SMILES: CCSc1ccoc1C
Mol. weight [g/mol]: 142.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.84		Crippen Method
logp	2.700		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
rinpol	1005.00		NIST Webbook
rinpol	1007.00		NIST Webbook
ripol	1388.00		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=R80625&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
rinpol: Non-polar retention indices
ripol: Polar retention indices