Furan, 3-(ethyldithio)-2-methyl

Other names: 3-(ethyldithio)-2-methylfuran
Inchi: InChI=1S/C7H10OS2/c1-3-9-10-7-4-5-8-6(7)2/h4-5H,3H2,1-2H3
InchiKey: ZPINLCXQMSVOQT-UHFFFAOYSA-N
Formula: C7H10OS2
SMILES: CCSSc1ccoc1C
Mol. weight [g/mol]: 174.28
CAS: 61197-07-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.72		Crippen Method
logp	3.348		Crippen Method
mcvol	128.600	ml/mol	McGowan Method
rinpol	1238.00		NIST Webbook
ripol	1725.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C61197077&Units=SI

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