

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

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