

Furfuryl isothiocyanate

Other names:	Furan, 2-(isothiocyanatomethyl)- 2-furfuryl isothiocyanate
Inchi:	InChI=1S/C6H5NOS/c9-5-7-4-6-2-1-3-8-6/h1-3H,4H2
InchiKey:	ICXYINJACKJQQV-UHFFFAOYSA-N
Formula:	C6H5NOS
SMILES:	S=C=NCc1ccco1
Mol. weight [g/mol]:	139.18
CAS:	4650-60-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.44		Crippen Method
logp	1.882		Crippen Method
mcvol	99.540	ml/mol	McGowan Method

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=C4650606&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/29-481-6/Furfuryl-isothiocyanate.pdf>

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