

2-Furfurylthiol

Other names:	2-Furanmethanethiol
	Furfuryl mercaptan
	Furfuryl thiol
	2-Furylmethanethiol
	2-Furylmethyl mercaptan
	«alpha»-Furfuryl mercaptan
	USAF B-58
	2-Furanmethanthiol
	2-Mercaptomethylfuran
	Furan-2-yl-methanethiol
Inchi:	InChI=1S/C5H6OS/c7-4-5-2-1-3-6-5/h1-3,7H,4H2
InchiKey:	ZFFTZDQKIXPDAF-UHFFFAOYSA-N
Formula:	C5H6OS
SMILES:	SCc1ccco1
Mol. weight [g/mol]:	114.17
CAS:	98-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.16		Crippen Method
logp	1.709		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
rinpol	911.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	883.00		NIST Webbook

rinpol	913.00	NIST Webbook
rinpol	883.00	NIST Webbook
rinpol	901.00	NIST Webbook
rinpol	888.00	NIST Webbook
rinpol	889.00	NIST Webbook
rinpol	887.00	NIST Webbook
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ripol	1427.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1436.00		NIST Webbook
tb	428.20	K	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=C98022&Units=SI

Legend

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

tb: Normal Boiling Point Temperature

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