

2-Methyl-3-furanthiol

Other names:	3-Furanthiol, 2-methyl- 2-Methyl, 3-furanethiol 2-Methyl-3-mercaptofuran 2-Methyl-3-sulfanylfuran 2-Methyl-furan-3-thiol Furan-3-thiol, 2-methyl
Inchi:	InChI=1S/C5H6OS/c1-4-5(7)2-3-6-4/h2-3,7H,1H3
InchiKey:	RUYNUXHHUVUINQ-UHFFFAOYSA-N
Formula:	C5H6OS
SMILES:	Cc1occc1S
Mol. weight [g/mol]:	114.17
CAS:	28588-74-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	1.877		Crippen Method
mcpvol	84.070	ml/mol	McGowan Method
rinpol	875.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	867.00		NIST Webbook

rinpol	879.00	NIST Webbook
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ripol	1300.00	NIST Webbook
ripol	1305.00	NIST Webbook
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ripol	1310.00	NIST Webbook
ripol	1305.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1341.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C28588741&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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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