

Ethanethioic acid, S-(2-furanylmethyl) ester

Other names:	Acetic acid, thio-, S-furfuryl ester Furfurylthiol acetate S-Furfuryl thioacetate S-furfuryl ethanethioate
Inchi:	InChI=1S/C7H8O2S/c1-6(8)10-5-7-3-2-4-9-7/h2-4H,5H2,1H3
InchiKey:	LQOUTUIIYXYBQW-UHFFFAOYSA-N
Formula:	C7H8O2S
SMILES:	CC(=O)SCc1ccco1
Mol. weight [g/mol]:	156.20
CAS:	13678-68-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.58		Crippen Method
logp	2.059		Crippen Method
mcvol	113.820	ml/mol	McGowan Method
rinpol	1163.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1769.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13678687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tbrp:	Boiling point at reduced pressure

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