

2,4-Thiazolidinedione, 5-(2-furfurylidene)-

Inchi:	InChI=1S/C8H5NO3S/c10-7-6(13-8(11)9-7)4-5-2-1-3-12-5/h1-4H,(H,9,10,11)/b6-4+
InchiKey:	OZIVFRZKBDVKEO-GQCTYLIASA-N
Formula:	C8H5NO3S
SMILES:	O=C1NC(=O)C(=Cc2ccco2)S1
Mol. weight [g/mol]:	195.19
CAS:	5718-88-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.86		Crippen Method
logp	1.603		Crippen Method
mcvol	124.300	ml/mol	McGowan Method

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=C5718887&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

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<https://www.chemeo.com/cid/36-340-4/2-4-Thiazolidinedione-5-2-furfurylidene.pdf>

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