

5-Furfurylidenebarbituric acid

Inchi:	InChI=1S/C9H6N2O4/c12-7-6(4-5-2-1-3-15-5)8(13)11-9(14)10-7/h1-4H,(H2,10,11,12,13,
InchiKey:	XDWMFQLVGXHUJV-UHFFFAOYSA-N
Formula:	C9H6N2O4
SMILES:	O=C1N=C(O)C(=Cc2ccco2)C(O)=N1
Mol. weight [g/mol]:	206.15
CAS:	27406-36-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	1.710		Crippen Method
mcvol	133.590	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27406366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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