

2-Furancarboxylic acid, morpholide

Inchi:	InChI=1S/C9H11NO3/c11-9(8-2-1-5-13-8)10-3-6-12-7-4-10/h1-2,5H,3-4,6-7H2
InchiKey:	MOZLMXOHIQAAND-UHFFFAOYSA-N
Formula:	C9H11NO3
SMILES:	O=C(c1ccco1)N1CCOCC1
Mol. weight [g/mol]:	181.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	0.752		Crippen Method
mcvol	130.640	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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