

2,4-Furandicarboxylic acid, dimethyl ester

Inchi:	InChI=1S/C8H8O5/c1-11-7(9)5-3-6(13-4-5)8(10)12-2/h3-4H,1-2H3
InchiKey:	GZNZEMZRQVMDDH-UHFFFAOYSA-N
Formula:	C8H8O5
SMILES:	<chem>COC(=O)c1coc(C(=O)OC)c1</chem>
Mol. weight [g/mol]:	184.15
CAS:	1710-13-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	0.853		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
rinpol	1365.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2153.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1710130&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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