

2,5-Furandicarboxylic acid, dimethyl ester

Other names: Dimethyl 2,5-furandicarboxylate
Furan-2,5-dicarboxylic acid dimethyl ester

Inchi: InChI=1S/C8H8O5/c1-11-7(9)5-3-4-6(13-5)8(10)12-2/h3-4H,1-2H3

InchiKey: UWQOPFRNDNVUOA-UHFFFAOYSA-N

Formula: C8H8O5

SMILES: COC(=O)c1ccc(C(=O)OC)o1

Mol. weight [g/mol]: 184.15

CAS: 4282-32-0

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	1346.00		NIST Webbook
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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=C4282320&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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