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: COC(=O)c1coc(C(=O)OC)c1
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