Furan-3-carboxylic acid, 5-ethyl-4-methyl-2-(2-methoxycarbonylethyl), methyl ester

Inchi: InChI=1S/C13H18O5/c1-5-9-8(2)12(13(15)17-4)10(18-9)6-7-11(14)16-3/h5-7H2,1-4H3
InchiKey: GOTXLXZJQJLBNQ-UHFFFAOYSA-N
Formula: C13H18O5
SMILES: CCc1oc(CCC(=O)OC)c(C(=O)OC)c1C
Mol. weight [g/mol]: 254.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.23		Crippen Method
logp	2.043		Crippen Method
mcvol	195.320	ml/mol	McGowan Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R106555&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.