

5-(Methoxycarbonylmethyl-carbamoyl)-furan-2-carboxylic acid methyl ester

InChI: COC(=O)CNC(=O)c1ccc(C(=O)OC)o1
InChIKey: ZNLNZQWJHIPKRQ-UHFFFAOYSA-N

Formula: C₁₀H₁₁NO₆

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

Mol. weight [g/mol]: 241.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	-0.031		Crippen Method
mcvol	164.600	ml/mol	McGowan Method
rinpol	1845.00		NIST Webbook

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=R247948&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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