

C11H9NO4

Inchi:	InChI=1S/C11H9NO4/c1-6(11(15)16)12-9(13)7-4-2-3-5-8(7)10(12)14/h2-6H,1H3,(H,15,1
InchiKey:	OZWUITKBAWTEAQ-LURJTMIESA-N
Formula:	C11H9NO4
SMILES:	CC(C(=O)O)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	219.19
CAS:	29588-83-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	0.756		Crippen Method
mcvol	151.790	ml/mol	McGowan Method

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=C29588838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/21-437-3/C11H9NO4.pdf>

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