

C13H13NO4

Inchi:	InChI=1S/C13H13NO4/c1-7(2)10(13(17)18)14-11(15)8-5-3-4-6-9(8)12(14)16/h3-7,10H,1
InchiKey:	UUIPGCXIZVZSEC-JTQLQIEISA-N
Formula:	C13H13NO4
SMILES:	CC(C)C(C(=O)O)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	247.25
CAS:	6306-54-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	1.392		Crippen Method
mcvol	179.970	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6306543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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/21-008-9/C13H13NO4.pdf>

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