

o-Toluic acid, morpholide

Other names:	o-Toluylic acid, morpholide
Inchi:	InChI=1S/C12H15NO2/c1-10-4-2-3-5-11(10)12(14)13-6-8-15-9-7-13/h2-5H,6-9H2,1H3
InchiKey:	PFKVDZHFKEKOEKV-UHFFFAOYSA-N
Formula:	C12H15NO2
SMILES:	<chem>Cc1ccccc1C(=O)N1CCOCC1</chem>
Mol. weight [g/mol]:	205.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.467		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
rinpola	1703.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307000&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/94-101-5/o-Toluic-acid-morpholide.pdf>

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