

Carbamic acid, n-(4-phthalimidobutyl)-n-(p-tolylsulfonyl)-, ethyl ester

Inchi:	InChI=1S/C22H24N2O6S/c1-3-30-22(27)24(31(28,29)17-12-10-16(2)11-13-17)15-7-6-14
InchiKey:	BCVIVDXQRUOTCI-UHFFFAOYSA-N
Formula:	C22H24N2O6S
SMILES:	CCOC(=O)N(CCCCN1C(=O)c2ccccc2C1=O)S(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	444.50
CAS:	15440-88-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	3.219		Crippen Method
mcvol	321.090	ml/mol	McGowan Method

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=C15440887&Units=SI

Legend

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

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