

P-toluenesulfonamide, n-(4-phthalimidobutyl)-

Inchi:	InChI=1S/C19H20N2O4S/c1-14-8-10-15(11-9-14)26(24,25)20-12-4-5-13-21-18(22)16-6-2
InchiKey:	ATMFSUWHIBENFU-UHFFFAOYSA-N
Formula:	C19H20N2O4S
SMILES:	<chem>Cc1ccc(S(=O)(=O)NCCCCN2C(=O)c3ccccc3C2=O)cc1</chem>
Mol. weight [g/mol]:	372.44
CAS:	15544-49-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	2.350		Crippen Method
mcvol	271.380	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=C15544497&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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