

Mefenacet

Other names:	2-(1,3-Benzothiazol-2-yloxy)-N-methyl-N-phenyl-acetamide 2-(benzothiazol-2-yloxy)-N-methyl-N-phenylacetamide
Inchi:	InChI=1S/C16H14N2O2S/c1-18(12-7-3-2-4-8-12)15(19)11-20-16-17-13-9-5-6-10-14(13)2
InchiKey:	XIGAUIHYSDTJHW-UHFFFAOYSA-N
Formula:	C16H14N2O2S
SMILES:	CN(C(=O)COc1nc2cccc2s1)c1cccc1
Mol. weight [g/mol]:	298.36
CAS:	73250-68-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.338		Crippen Method
mcpol	217.370	ml/mol	McGowan Method
rinpol	2566.00		NIST Webbook
rinpol	2575.00		NIST Webbook
rinpol	2613.00		NIST Webbook
rinpol	2588.00		NIST Webbook
rinpol	2566.00		NIST Webbook
rinpol	2613.00		NIST Webbook
rinpol	2566.00		NIST Webbook
rinpol	2588.00		NIST Webbook

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=C73250687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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