

Bentazon methyl

Other names:	Bentazone, methylated Bentazone, methyl ester Bentazon methyl ester N-Methylbentazon
Inchi:	InChI=1S/C11H14N2O3S/c1-8(2)13-11(14)9-6-4-5-7-10(9)12(3)17(13,15)16/h4-8H,1-3H
InchiKey:	XFTQFXBQDVWOCY-UHFFFAOYSA-N
Formula:	C11H14N2O3S
SMILES:	<chem>CC(C)N1C(=O)c2ccccc2N(C)S1(=O)=O</chem>
Mol. weight [g/mol]:	254.31
CAS:	61592-45-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.232		Crippen Method
mvol	180.850	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=C61592458&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
mvol:	McGowan's characteristic volume

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