

pyributicarb

Other names:	Carbamothioic acid, N-(6-methoxy-2-pyridinyl)-N-methyl-, O-[3-(1,1-dimethylethyl)phenyl] ester
Inchi:	InChI=1S/C18H22N2O2S/c1-18(2,3)13-8-6-9-14(12-13)22-17(23)20(4)15-10-7-11-16(19)
InchiKey:	VTRWMTJQBQJKQH-UHFFFAOYSA-N
Formula:	C18H22N2O2S
SMILES:	COc1cccc(N(C)C(=S)Oc2cccc(C(C)(C)C)c2)n1
Mol. weight [g/mol]:	330.44
CAS:	88678-67-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	4.188		Crippen Method
mcvol	260.710	ml/mol	McGowan Method
rinpol	2426.00		NIST Webbook
rinpol	2436.00		NIST Webbook
rinpol	2426.00		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=C88678675&Units=SI

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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