

Pirimicarb

Other names:	2-(Dimethylamino)-5,6-dimethyl-4-pyrimidinyl dimethylcarbamate 2-Dimethylamino-5,6-dimethylpyrimidin-4-yl dimethylcarbamate 5,6-Dimethyl-2-dimethylamino-4-dimethylcarbamoyloxy pyrimidine 5,6-Dimethyl-2-dimethylamino-4-pyrimidinyl dimethylcarbamate Abol Aficida Aphox Carbamic acid, dimethyl-, 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester Carbamic acid, dimethyl-, 2-(dimethylamino)-5,6-dimethyl-4-pyrimidyl ester Dimethylcarbamic acid 2-(dimethylamino)-5,6-dimethyl-4-pyrimidinyl ester ENT-27766 Fernos OMS 1330 PP 062 Pirimicarbe Pirimor Pirimor G Pirimor granulate Primicarbe Pyrimicarbe Pyrimor Rapid
Inchi:	InChI=1S/C11H18N4O2/c1-7-8(2)12-10(14(3)4)13-9(7)17-11(16)15(5)6/h1-6H3
InchiKey:	YFGYUFNIOHWBOB-UHFFFAOYSA-N
Formula:	C11H18N4O2
SMILES:	<chem>Cc1nc(N(C)C)nc(OC(=O)N(C)C)c1C</chem>
Mol. weight [g/mol]:	238.29
CAS:	23103-98-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Estimated Solubility Method
log10ws	-1.95		Aqueous Solubility Prediction Method
logp	1.220		Crippen Method
mcvol	189.450	ml/mol	McGowan Method

rmpol	1813.00		NIST Webbook
rmpol	1837.00		NIST Webbook
rmpol	1816.00		NIST Webbook
rmpol	1836.00		NIST Webbook
rmpol	1840.00		NIST Webbook
rmpol	1839.00		NIST Webbook
rmpol	1837.00		NIST Webbook
rmpol	1866.00		NIST Webbook
rmpol	1796.00		NIST Webbook
rmpol	1836.00		NIST Webbook
rmpol	1837.00		NIST Webbook
rmpol	1816.00		NIST Webbook
rmpol	1839.00		NIST Webbook
rmpol	1816.00		NIST Webbook
rmpol	1810.00		NIST Webbook
rmpol	1807.00		NIST Webbook
rmpol	1796.00		NIST Webbook
tf	363.65	K	Aqueous Solubility Prediction Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C23103982&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Estimated Solubility Method:

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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