

Pirimicarb-desmethyl

Other names:

Carbamic acid, dimethyl-, 5,6-dimethyl-2-(methylamino)-4-pyrimidinyl ester
5,6-Dimethyl-2-(methylamino)-4-pyrimidinyl dimethylcarbamate
Desmethylpirimicarb
Pyrimidin-4-ol, 2-methylamino, 5,6-dimethyl, N,N-dimethylcarbamate
Pirimicarb demethyl

Inchi:

InChI=1S/C10H16N4O2/c1-6-7(2)12-9(11-3)13-8(6)16-10(15)14(4)5/h1-5H3,(H,11,12,13)

InchiKey:

GTKRZJVAXAQBMB-UHFFFAOYSA-N

Formula:

C10H16N4O2

SMILES:

CNc1nc(C)c(C)c(OC(=O)N(C)C)n1

Mol. weight [g/mol]:

224.26

CAS:

30614-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.196		Crippen Method
mcvol	175.360	ml/mol	McGowan Method

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C30614223&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

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