

PYRIMETHANIL

Other names:	2-Pyrimidinamine, 4,6-dimethyl-N-phenyl- 2-anilino-4,6-dimethylpyrimidine 4,6-Dimethyl-N-phenyl-2-pyrimidinamine 4,6-Dimethyl-N-phenyl-pyrimidin-2-amine 4,6-dimethyl-N-phenylpyrimidin-2-amine
Inchi:	InChI=1S/C12H13N3/c1-9-8-10(2)14-12(13-9)15-11-6-4-3-5-7-11/h3-8H,1-2H3,(H,13,14,
InchiKey:	ZLIBICFPKPWGIZ-UHFFFAOYSA-N
Formula:	C12H13N3
SMILES:	Cc1cc(C)nc(Nc2ccccc2)n1
Mol. weight [g/mol]:	199.25
CAS:	53112-28-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	2.837		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
rinpol	1813.00		NIST Webbook
rinpol	1789.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tf	369.29	K	Measurement and Correlation of the Solubility of Pyrimethanil in Seven Monosolvents and Two Different Binary Mixed Solvents

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.23	kJ/mol	234.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation of the Solubility of Pyrimethanil in Seven	https://www.doi.org/10.1021/acs.jced.8b00124
McGowan Method	http://link.springer.com/article/10.1007/BF02311772
Non-Solvents and Two Different Binary Mixed Solvents:	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53112280&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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