

Pyridate

Other names:	Carbonothioic acid, O-(6-chloro-3-phenyl-4-pyridazinyl) S-octyl ester O-(6-Chloro-3-phenyl-4-pyridazinyl) S-octyl carbonothioate CL 11344 Fenpyrate Lentagran P1 3419 Pyron Tough O-(6-Chloro-3-phenyl-4-pyridazinyl) S-octyl thiocarbonate O-(6-chloro-3-phenylpyridazin-4-yl) S-octyl thiocarbonate
Inchi:	InChI=1S/C19H23ClN2O2S/c1-2-3-4-5-6-10-13-25-19(23)24-16-14-17(20)21-22-18(16)1
InchiKey:	JTZCTMAVMHRNTR-UHFFFAOYSA-N
Formula:	C19H23ClN2O2S
SMILES:	CCCCCCCCSC(=O)Oc1cc(Cl)nnc1-c1cccc1
Mol. weight [g/mol]:	378.92
CAS:	55512-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.40		Crippen Method
logp	6.389		Crippen Method
mcvol	287.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55512339&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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