Crufomate

Other names:	Phosphoramidic acid, methyl-, 2-chloro-4-(1,1-dimethylethyl)phenyl methyl ester
	Phosphoramidic acid, methyl-, 4-tert-butyl-2-chlorophenyl methyl ester
	Amidofos
	Amidophos
	Crufomat
	Dowco 132
	Montrel
	Ruelene
	Ruelene drench
	4-tert-Butyl-2-Chlorophenyl methyl methylphosphoramidate
	o-(4-tert-Butyl-2-chlor-phenyl)-O-methyl-phosphorsaeure-N-methylamid
	Cruformate
	ENT 25,602-x
	Methylphosphoramidic acid, 4-tert-butyl-2-chlorophenyl methyl ester
	N,O-Dimethyl-o-(4-tert-butyl-2-chlorophenyl)phosphoramidate
	O-(4-tert Butyl-2-chloor-fenyl)-O-methyl-fosforzuur-N-methyl-amide
	O-(4-Terz.-butil-2-cloro-fenil)-O-metil-fosforammide
	O-Methyl O-2-chloro-4-tert-butylphenyl N-methylamidophosphate
	Phenol, 4-tert-butyl-2-chloro-, ester with methyl methylphosphoramidate
	Rulene
	4-tert-Butyl-2-chlorophenyl O-methyl methylphosphoroamidate
	4-t-Butyl-2-chlorophenyl methyl methylphosphoramidate
	Crufomate A
	M-1261
	Methylphosphoramidic acid, 4-t-butyl-2-chlorophenyl methyl ester
	Phenol, 4-t-butyl-2-chloro-, ester with methyl methylphosphoramidate
	Phosphoramidic acid, 4-tert-butyl-2-chlorophenylphosphoramidate
	Ruelene 25E
	O-(4-tert-Butyl-2-chlorophenyl) O-methyl N-methylamido phosphate
	NSC 253463
	N-methyl O-methyl O-2-chloro-4-tert-butylphenylphosphoramidate
Inchi:	InChI=1S/C12H19ClNO3P/c1-12(2,3)9-6-7-11(10(13)8-9)17-18(15,14-4)16-5/h6-8H,1-5H
InchiKey:	BOFHKBLZOYVHSI-UHFFFAOYSA-N
Formula:	C12H19ClNO3P
SMILES:	CNP(=O)(OC)Oc1ccc(C(C)(C)C)cc1Cl
Mol. weight [g/mol]:	291.71
CAS:	299-86-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	3.990		Crippen Method
mcvol	216.470	ml/mol	McGowan Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tf	333.29 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.98	kJ/mol	332.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C299865&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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