Phosphamidon

Other names:

Phosphoric acid, 2-chloro-3-(diethylamino)-1-methyl-3-oxo-1-propenyl dimethyl ester
Phosphoric acid, dimethyl ester, ester with 2-chloro-N,N-diethyl-3-hydroxycrotonamide
Dimecron
Dimecron 100
Dimecron 50
Dimecron-20
Merkon
Phosphamidone
Sundaram 1975
Apamidon
C 570
(2-Chloor-3-diethylamino-1-methyl-3-oxo-prop-1-en-yl)-dimethyl-fosfaat
(2-Chlor-3-diaethylamino-1-methyl-3-oxo-prop-1-en-yl)-dimethyl-phosphat
2-Chloro-2-diethylcarbamoyl-1-methylvinyl dimethylphosphate
1-Chloro-diethylcarbamoyl-1-propen-2-yl dimethyl phosphate
(2-Cloro-3-dietilamino-1-metil-3-oxo-prop-1-en-il)-dimetil-fosfato
Ciba 570
Crotonamide, 2-chloro-N,N-diethyl-3-hydroxy-, dimethyl phosphate
Dimethyl 2-chloro-2-diethylcarbamoyl-1-methylvinyl phosphate
O,O-Dimethyl O-(2-chloro-2-(N,N-diethylcarbamoyl)-1-methylvinyl) phosphate
Dimethyl diethylamido-1-chlorocrotonyl (2) phosphate
O,O-Dimethyl-O-(1-methyl-2-chlor-2-N,N-diaethyl-carbamoyl)-vinyl-phosphat
(O,O-Dimethyl-O-(1-methyl-2-chloro-2-diethylcarbamoyl-vinyl) phosphate)
Dimethyl phosphate of 2-chloro-N,N-diethyl-3-hydroxycrotonamide
Dixon
ENT 25515
Famfos
Fosfamidon
Fosfamidone
ML 97
NCI-C00588
OMS 1325
OR 1191
Foszfamidon
2-Chloro-3-(diethylamino)-1-methyl-3-oxo-1-propenyl dimethyl phosphate
Phosphamidon II
Phosphamidon I

Inchi: InChI=1S/C10H19ClNO5P/c1-6-12(7-2)10(13)9(11)8(3)17-18(14,15-4)16-5/h6-7H2,1-5H

InchiKey: RGCLLPNLLBQHPF-HJWRWDBZSA-N

Formula: C10H19ClNO5P

SMILES: CCN(CC)C(=O)C(Cl)=C(C)OP(=O)(OC)OC
Mol. weight [g/mol]: 299.69
CAS: 13171-21-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	2.743		Crippen Method
mcvol	215.190	ml/mol	McGowan Method
rinpol	1860.00		NIST Webbook
rinpol	1833.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1825.00		NIST Webbook
ripol	2831.00		NIST Webbook
ripol	2831.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	90.10	kJ/mol	340.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13171216&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvapt:	Enthalpy of vaporization 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
ripol:	Polar retention indices