

Butamifos

Other names:

Phosphoramidothioic acid, N-(sec-butyl)-, O-ethyl O-(6-nitro-m-tolyl) ester
Cremart
O-Ethyl O-(3-methyl-6-nitrophenyl) N-sec-butylphosphorothioamidate
O-Ethyl-O-(5-methyl-2-nitrophenyl)(1-methylpropyl)phosphoramidothioate
H 26905
Hercules 26905
Kremart
Metacrefos
Phosphoramidothioic acid, (1-methylpropyl)-, O-ethyl O-(5-methyl-2-nitrophenyl) ester
S 28
S 2846
S 28 (pesticide)
Phosphoramidothioic acid, N-(1-methylpropyl)-, O-ethyl O-(5-methyl-2-nitrophenyl) ester

Inchi:

InChI=1S/C13H21N2O4PS/c1-5-11(4)14-20(21,18-6-2)19-13-9-10(3)7-8-12(13)15(16)17

InchiKey:

OEYOMNZEMCPTKN-UHFFFAOYSA-N

Formula:

C13H21N2O4PS

SMILES:

CCOP(=S)(NC(C)CC)Oc1cc(C)ccc1[N+](=O)[O-]

Mol. weight [g/mol]:

332.36

CAS:

36335-67-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.45		Crippen Method
logp	3.931		Crippen Method
mcvol	246.220	ml/mol	McGowan Method
rinpol	2138.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2190.90		NIST Webbook
rinpol	2178.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36335678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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
rinpola:	Non-polar retention indices

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