Iprobenfos

Other names:	Kitazin P
	Phosphorothioic acid, O,O-bis(1-methylethyl) S-(phenylmethyl) ester
	Phosphorothioic acid, S-benzyl O,O-diisopropyl ester
	IBP
	Kitazin L
	O,O-Diisopropyl S-Benzyl phosphorothioate
	O,O-Diisopropyl S-benzyl thiophosphate
	S-Benzyl O,O-diisopropyl phosphorothioate
	S-Benzyl O,O-diisopropyl thiophosphate
	Iprofenfos
	O,O-Diisopropyl S-benzyl phosphorothiolate
	Ricid II
	Ricid P
	S-benzyl diisopropyl phosphorothioate
Inchi:	InChI=1S/C13H21O3PS/c1-11(2)15-17(14,16-12(3)4)18-10-13-8-6-5-7-9-13/h5-9,11-12H
InchiKey:	FCOAHACKGGIURQ-UHFFFAOYSA-N
Formula:	C13H21O3PS
SMILES:	CC(C)OP(=O)(OC(C)C)SCc1ccccc1
Mol. weight [g/mol]:	288.34
CAS:	26087-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	4.878		Crippen Method
mcvol	224.690	ml/mol	McGowan Method
rinpol	1838.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1838.00		NIST Webbook

ripol	2534.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.00	K	0.01	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26087478&Units=SI
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

Legend

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
tbrp:	Boiling point at reduced pressure