Quinalphos

Other names:	Phosphorothioic acid, O,O-diethyl O-2-quinoxalinyl ester
	Bayer 77049
	Bayrusil
	BAY 77049
	Diethchinalphion
	Diethyl 2-Quinoxalyl phosphorothionate
	Ekalux
	O,O-Diethyl O-(quinoxalin-2-yl) thiophosphate
	O,O-Diethyl O-(2-quinoxalyl) phosphorothionate
	Quinolphos
	Sandoz 6538
	Sandoz 6626
	SAN 6538
	SAN 6626
	Diethquinalphion
	Diethyl O-(2-quinoxalyl) phosphorothioate
	Diethyl O-(quinoxalin-2-yl) thiophosphate
	Diethyl O-2-quinoxalinyl phosphorothioate
	Diethyl O-quinoxalin-2-yl thionophosphate
	O,O-Diethyl O-2-quinoxalinyl phosphorothioate
	Savall
	SRA 7312
	Wie oben
	Quinaltaf
	O,O-diethyl O-quinoxalin-2-yl phosphothioate
Inchi:	InChI=1S/C12H15N2O3PS/c1-3-15-18(19,16-4-2)17-12-9-13-10-7-5-6-8-11(10)14-12/h5-
InchiKey:	JYQUHIFYBATCCY-UHFFFAOYSA-N
Formula:	C12H15N2O3PS
SMILES:	CCOP(=S)(OCC)Oc1cnc2ccccc2n1
Mol. weight [g/mol]:	298.30
CAS:	13593-03-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.61		Crippen Method
logp	3.306		Crippen Method

mcvol	211.100	ml/mol	McGowan Method
rinpol	2067.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2086.00		NIST Webbook
tf	304.48 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.40	kJ/mol	304.10	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=C13593038&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