Phosphorothioic acid, O,O-diethyl O-2-quinoxalinyl ester

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

Physical Properties

Property code	Value	Unit	Source
ie	8.40	eV	Cheméo Relay (1.0)
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
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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13593038&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hfust: Enthalpy of fusion at a given temperature
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point