Phosphorothioic acid, O-(4-aminophenyl) O,O-diethyl ester

Other names: E 605 Reduced
O,O-Diethyl O-(4-aminophenyl) phosphorothioate
O-(4-Aminophenyl) O,O-diethyl phosphorothioate
Phosphorothioic acid, O-(4-aminophenyl) O,O-diethyl ester
Phosphorothioic acid, O-(p-aminophenyl) O,O-diethyl ester
p-Aminoparathion

Inchi: InChI=1S/C10H16NO3PS/c1-3-12-15(16,13-4-2)14-10-7-5-9(11)6-8-10/h5-8H,3-4,11H2,

InchiKey: XIZOTXGJXSTQDI-UHFFFAOYSA-N

Formula: C10H16NO3PS

SMILES: CCOP(=S)(OCC)Oc1ccc(N)cc1

Mol. weight [g/mol]: 261.28

Physical Properties

Property code	Value	Unit	Source
ie	7.36	eV	Cheméo Relay (1.0)
log10ws	-3.35		Cheméo Relay (1.0)
logp	2.945		Crippen Method
mcvol	192.400	ml/mol	McGowan Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	628.28	K	Cheméo Relay (1.0)
tf	293.78	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3735011&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point