AMITON

Other names: O,O-Diethyl S-[2-diethylaminoethyl]phosphorothioate
Phosphorothioic acid, S-(2-(diethylamino)ethyl) O,O-diethyl ester
Chipman 6200
S-(Diethylaminoethyl) O,O-diethyl phosphorothioate
S-(2-(Diethylamino)ethyl)phosphorothioic acid O,O-diethyl ester
(2-Diethylamino)ethylphosphorothioic acid O,O-diethyl ester
O,O-Diethyl-S-2-(diethylamino)ethylester kyseliny thiofosforecne
Diethyl S-2-diethylaminoethyl phosphorothioate
O,O-Diethyl S-diethylaminoethyl phosphorothioate
O,O-Diethyl S-(«beta»-diethylamino)ethyl phosphorothioate
O,O-Diethyl S-(2-diethylaminoethyl) thiophosphate
DSDP
ENT 24,980-X
Inferno
Metramac
Metramak
R-5,158
Rhodia-6200
Tetram
O,O-Diethyl S-2-diethylaminoethyl phosphorothiolate
R 5158
VG
VG (chemical warfare agent)

Inchi: InChI=1S/C10H24NO3PS/c1-5-11(6-2)9-10-16-15(12,13-7-3)14-8-4/h5-10H2,1-4H3

InchiKey: PJISLFCKHOHLLP-UHFFFAOYSA-N

Formula: C10H24NO3PS

SMILES: CCOP(=O)(OCC)SCCN(CC)CC

Mol. weight [g/mol]: 269.35

Physical Properties

Property code	Value	Unit	Source
hvap	73.93	kJ/mol	Cheméo Relay (1.0)
ie	8.29	eV	Cheméo Relay (1.0)
log10ws	-1.08		Cheméo Relay (1.0)
logp	3.243		Crippen Method
mcvol	216.160	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78535&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):	

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume