Cythioate

Other names: Phosphorothioic acid, O-[4-(aminosulfonyl)phenyl] O,O-dimethyl ester
Phosphorothioic acid, O,O-dimethyl ester, O-ester with p-hydroxybenzenesulfonamide
American Cyanamid CL-26,691
Benzenesulfonamide, p-hydroxy-, O-ester with O,O-dimethyl phosphorothioate
Cyflee
CL 26691
ENT 25,640
O,O-Dimethyl O-p-Sulfamoylphenyl phosphorothioate
Proban
American CL-26,691
AC 26,691
American CL-26691
O-(4-(Aminosulfonyl)phenyl) O,O-dimethyl phosphorothioate
NSC 310287
O,O-dimethyl O-(4-sulphamoylphenyl) thiophosphate
O,O-dimethyl O-(4-aminosulfonylphenyl)phosphorodithioate

Inchi: InChI=1S/C8H12NO5PS2/c1-12-15(16,13-2)14-7-3-5-8(6-4-7)17(9,10)11/h3-6H,1-2H3,(H
InchiKey: BSBSDQUZDZXGFN-UHFFFAOYSA-N
Formula: C8H12NO5PS2
SMILES: COP(=S)(OC)Oc1ccc(S(N)(=O)=O)cc1
Mol. weight [g/mol]: 297.29
CAS: 115-93-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.86		Crippen Method
logp	1.230		Crippen Method
mcvol	192.310	ml/mol	McGowan Method
tf	345.67 ± 0.20	K	NIST Webbook
tf	347.00 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hfust	26.21	kJ/mol	344.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115935&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

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
tf:	Normal melting (fusion) point