

Phosphorothioic acid, s-ester with n-[4-[(3-hydroxypropyl)amino]butyl]phthalimide

Inchi:	InChI=1S/C15H21N2O5PS/c18-14-12-6-1-2-7-13(12)15(19)17(14)10-4-3-8-16-9-5-11-24
InchiKey:	XTLLEHXVVHCTOQ-UHFFFAOYSA-N
Formula:	C15H21N2O5PS
SMILES:	O=C1c2ccccc2C(=O)N1CCCCNCCCSP(=O)(O)O
Mol. weight [g/mol]:	372.38
CAS:	31786-68-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.20		Crippen Method
logp	1.868		Crippen Method
mcvol	265.110	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C31786682&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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