

Trichlorophenyl cyclohexylamido ethyl thiophosphate

Inchi:	InChI=1S/C14H19Cl3NO2PS/c1-2-19-21(22,18-10-6-4-3-5-7-10)20-14-9-12(16)11(15)8-
InchiKey:	BNWPHCMSAUZTRF-UHFFFAOYSA-N
Formula:	C14H19Cl3NO2PS
SMILES:	CCOP(=S)(NC1CCCCC1)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	402.70
CAS:	116295-49-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	6.209		Crippen Method
mcvol	268.750	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295499&Units=SI
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

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/123-244-4/Trichlorophenyl-cyclohexylamido-ethyl-thiophosphate.pdf>

Generated by Cheméo on 2024-04-28 09:10:17.495967244 +0000 UTC m=+16584666.416544565.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.