triclofos

Inchi: InChI=1S/C2H4Cl3O4P/c3-2(4,5)1-9-10(6,7)8/h1H2,(H2,6,7,8)
InchiKey: YYQRGCZGSFRBAM-UHFFFAOYSA-N
Formula: C2H4Cl3O4P
SMILES: O=P(O)(O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 229.38
CAS: 306-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.466		Crippen Method
mcvol	119.700	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C306525&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

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