

Dioxathion degradation product

Inchi:	InChI=1S/C8H15O4PS2/c1-3-11-13(14,12-4-2)15-8-7-9-5-6-10-8/h7H,3-6H2,1-2H3
InchiKey:	BRKIRWVYJPUKQJ-UHFFFAOYSA-N
Formula:	C8H15O4PS2
SMILES:	CCOP(=S)(OCC)SC1=COCCO1
Mol. weight [g/mol]:	270.31

Physical Properties

Property code	Value	Unit	Source
log10ws	1.11		Crippen Method
logp	2.863		Crippen Method
mcvol	185.060	ml/mol	McGowan Method
rinsol	1795.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/30-196-1/Dioxathion-degradation-product.pdf>

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