

Ibp

Inchi: InChI=1S/C11H17O3PS/c1-3-13-15(12,14-4-2)16-10-11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-
InchiKey: XFMJUIKWKVJNDY-UHFFFAOYSA-N
Formula: C11H17O3PS
SMILES: CCOP(=O)(OCC)SCc1ccccc1
Mol. weight [g/mol]: 260.29
CAS: 13286-32-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	4.101		Crippen Method
mcvol	196.510	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.50 ± 2.50	K	0.30	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=C13286323&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure

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<https://www.chemeo.com/cid/24-063-5/lbp.pdf>

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