

Bromodifluoromethyl diethylphosphonate

Inchi: InChI=1S/C5H10BrF2O3P/c1-3-10-12(9,11-4-2)5(6,7)8/h3-4H2,1-2H3
InchiKey: QRADKVYIJAENZ-UHFFFAOYSA-N
Formula: C5H10BrF2O3P
SMILES: CCOP(=O)(OCC)C(F)(F)Br
Mol. weight [g/mol]: 267.01
CAS: 65094-22-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	3.198		Crippen Method
mcpvol	140.420	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.50 ± 1.50	K	2.10	NIST Webbook

Sources

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=C65094226&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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