Ifosfamide

Inchi: InChI=1S/C7H15Cl2N2O2P/c8-2-4-10-14(12)11(6-3-9)5-1-7-13-14/h1-7H2,(H,10,12)
InchiKey: HOMGKSMUEGBAAB-UHFFFAOYSA-N
Formula: C7H15Cl2N2O2P
SMILES: O=P1(NCCCl)OCCCN1CCCl
Mol. weight [g/mol]: 261.09
CAS: 3778-73-2

Physical Properties

Property code	Value	Unit	Source
logp	1.884		Crippen Method
mcvol	175.270	ml/mol	McGowan Method
tf	315.90	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/107-189-4/Ifosfamide.pdf

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