

Ionidamine

Inchi: InChI=1S/C15H10Cl2N2O2/c16-10-6-5-9(12(17)7-10)8-19-13-4-2-1-3-11(13)14(18-19)15
InchiKey: WDRYRZXSPDWGEB-UHFFFAOYSA-N
Formula: C15H10Cl2N2O2
SMILES: O=C(O)c1nn(Cc2ccc(Cl)cc2Cl)c2ccccc12
Mol. weight [g/mol]: 321.16
CAS: 50264-69-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.03		Crippen Method
logp	4.090		Crippen Method
mccvol	211.410	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	45.92	kJ/mol	480.20	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=C50264692&Units=SI&Mask=3FFF>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hfust: Enthalpy of fusion at a given temperature

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

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