

Isoxazole-5-carbonyl chloride

Inchi: InChI=1S/C4H2ClNO2/c5-4(7)3-1-2-6-8-3/h1-2H
InchiKey: NASLINFISOTVJJ-UHFFFAOYSA-N
Formula: C4H2ClNO2
SMILES: O=C(Cl)c1ccno1
Mol. weight [g/mol]: 131.52
CAS: 62348-13-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.86		Crippen Method
logp	1.054		Crippen Method
mcvol	77.420	ml/mol	McGowan Method
rinpol	918.00		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=C62348134&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

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<https://www.chemeo.com/cid/60-350-6/Isoxazole-5-carbonyl-chloride.pdf>

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