

Isoxazole-5-carbonyl chloride

InChI: InChI=1S/C4H2ClNO2/c5-4(7)3-1-2-6-8-3/h1-2H

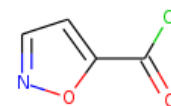
InChI Key: NASLINFISOTVJJ-UHFFFAOYSA-N

Formula: C4H2ClNO2

SMILES: O=C(Cl)c1ccno1

Molecular Weight: 131.52

CAS: 62348-13-4



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	1.054		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C4H2ClNO2/c5-4\(7\)3-1-2-6-8-3/h1-2H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C4H2ClNO2/c5-4(7)3-1-2-6-8-3/h1-2H)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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