5-Nitro-2-furoyl chloride

Other names:	2-Furancarbonyl chloride, 5-nitro- 2-Furoyl chloride, 5-nitro- 5-nitrofuroyl chloride
Inchi:	InChI=1S/C5H2ClNO4/c6-5(8)3-1-2-4(11-3)7(9)10/h1-2H
InchiKey:	OLEFNFXYGGTROA-UHFFFAOYSA-N
Formula:	C5H2ClNO4
SMILES:	O=C(Cl)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]:	175.53
CAS:	25084-14-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.75		Crippen Method
logp	1.567		Crippen Method
mcvol	98.950	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25084144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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