

5-Nitrothiophene-2-aldehyde

Other names:	5-Nitro 2-thiophenecarboxaldehyde 5-Nitrothiophene-2-carboxaldehyde 2-Thiophenecarboxaldehyde, 5-nitro- Thiophenecarboxaldehyde, 5-nitro- 5-nitrothiophene-2-carbaldehyde
Inchi:	InChI=1S/C5H3NO3S/c7-3-4-1-2-5(10-4)6(8)9/h1-3H
InchiKey:	CHTSWZNXEKOLPM-UHFFFAOYSA-N
Formula:	C5H3NO3S
SMILES:	O=Cc1ccc([N+](=O)[O-])s1
Mol. weight [g/mol]:	157.15
CAS:	4521-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.469		Crippen Method
mcvol	97.190	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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