

3,5-Dimethylisoxazole-4-carboxylic acid

Other names:	4-Isoxazolecarboxylic acid, 3,5-dimethyl-
Inchi:	InChI=1S/C6H7NO3/c1-3-5(6(8)9)4(2)10-7-3/h1-2H3,(H,8,9)
InchiKey:	IJEUISLJVBUNRE-UHFFFAOYSA-N
Formula:	C6H7NO3
SMILES:	Cc1noc(C)c1C(=O)O
Mol. weight [g/mol]:	141.12
CAS:	2510-36-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Crippen Method
logp	0.990		Crippen Method
mcvol	99.230	ml/mol	McGowan Method

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=C2510363&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/15-839-4/3-5-Dimethylisoxazole-4-carboxylic-acid.pdf>

Generated by Cheméo on 2024-04-27 02:41:34.766411522 +0000 UTC m=+16474943.686988839.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.