

4-Pyrazolecarboxylic acid, 5-amino-, methyl ester

Inchi:	InChI=1S/C5H7N3O2/c1-10-5(9)3-2-7-8-4(3)6/h2H,1H3,(H3,6,7,8)
InchiKey:	KGQFAPZUQKYADG-UHFFFAOYSA-N
Formula:	C5H7N3O2
SMILES:	COC(=O)c1cn[nH]c1N
Mol. weight [g/mol]:	141.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.33		Crippen Method
logp	-0.703		Crippen Method
mcvol	99.230	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6010403&Units=SI

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.cheméo.com/cid/115-113-8/4-Pyrazolecarboxylic-acid-5-amino-methyl-ester.pdf>

Generated by Cheméo on 2024-04-29 20:21:48.384123707 +0000 UTC m=+16711357.304701019.

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