

Ethyl 5-amino-1-methylpyrazole-4-carboxylate

Other names:	1H-Pyrazole-4-carboxylic acid, 5-amino-1-methyl-, ethyl ester Pyrazole-4-carboxylic acid, 5-amino-1-methyl-, ethyl ester 5-Amino-1-methylpyrazole-4-carboxylic acid ethyl ester Ethyl 3-amino-1-methylpyrazole-4-carboxylate Ethyl 5-amino-1-methyl-4-pyrazolecarboxylate Ethyl 1-methyl-5-aminopyrazole-4-carboxylate
Inchi:	InChI=1S/C7H11N3O2/c1-3-12-7(11)5-4-9-10(2)6(5)8/h4H,3,8H2,1-2H3
InchiKey:	MEUSJJFWVKBUFP-UHFFFAOYSA-N
Formula:	C7H11N3O2
SMILES:	CCOC(=O)c1cnn(C)c1N
Mol. weight [g/mol]:	169.18
CAS:	31037-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	0.179		Crippen Method
mcvol	127.410	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=C31037022&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

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