

Ethyl 4-pyrazolecarboxylate

Other names:	Ethyl 1H-pyrazole-4-carboxylate Pyrazole-4-carboxylic acid, ethyl ester 1H-Pyrazole-4-carboxylic acid, ethyl ester 4-(C ₂ H ₅ COO)-pyrazole
Inchi:	InChI=1S/C6H8N2O2/c1-2-10-6(9)5-3-7-8-4-5/h3-4H,2H2,1H3,(H,7,8)
InchiKey:	KACZQOKEFKFNDB-UHFFFAOYSA-N
Formula:	C ₆ H ₈ N ₂ O ₂
SMILES:	CCOC(=O)c1cn[nH]c1
Mol. weight [g/mol]:	140.14
CAS:	37622-90-5

Physical Properties

Property code	Value	Unit	Source
affp	880.70	kJ/mol	NIST Webbook
basg	846.50	kJ/mol	NIST Webbook
log10ws	-1.12		Crippen Method
logp	0.104		Crippen Method
mvol	103.340	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=C37622905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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