

1H-Pyrazole-4-carboxaldehyde, 1,5-dimethyl-

Other names:	Pyrazole-4-carboxaldehyde, 1,5-dimethyl- 1,5-Dimethyl-1H-pyrazole-4-carbaldehyde
Inchi:	InChI=1S/C6H8N2O/c1-5-6(4-9)3-7-8(5)2/h3-4H,1-2H3
InchiKey:	SGNRGSSHBKIJR-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	Cc1c(C=O)cnn1C
Mol. weight [g/mol]:	124.14
CAS:	25711-30-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	0.541		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1047.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25711302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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