1H-Pyrrole-2-carboxaldehyde, 5-methyl-

Other names:	2-Formyl-5-methylpyrrole
	5-methyl-1H-pyrrole-2-carboxaldehyde
	5-Methyl-2-formylpyrrole
	5-Methyl-2-pyrrolaldehyde
	5-Methylpyrrole-2-carboxaldehyde
	Pyrrole-2-carboxaldehyde, 5-methyl
	5-methyl-(1H)-pyrrole-2-carbaldehyde
Inchi:	InChI=1S/C6H7NO/c1-5-2-3-6(4-8)7-5/h2-4,7H,1H3
InchiKey:	LFWLUDLUCDRDAF-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Cc1ccc(C=O)[nH]1
Mol. weight [g/mol]:	109.13
CAS:	1192-79-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	0.654		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
rinpol	1092.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1099.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2079.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1192796&Units=SI

Legend

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