1H-Pyrrole-2-carboxaldehyde, 1-ethyl-

Other names:	1-Ethyl-1H-pyrrole-2-carboxaldehyde
	1-Ethyl-1H-pyrrole-2-carboxyaldehyde
	1-Ethyl-2-formyl-1H-pyrrole
	1-Ethyl-2-formylpyrrole
	1-Ethyl-2-pyrrolecarbaldehyde
Inchi:	InChI=1S/C7H9NO/c1-2-8-5-3-4-7(8)6-9/h3-6H,2H2,1H3
InchiKey:	DVLGEHCERRWDIX-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	CCn1cccc1C=O
Mol. weight [g/mol]:	123.15
CAS:	2167-14-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.321		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
rinpol	1046.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1067.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1610.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2167148&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices