

Methyl 1-methylpyrrole-2-carboxylate

Other names:	2-(methoxycarbonyl)-1-methylpyrrole 2-methoxycarbonyl-N-methylpyrrole methyl 1-methyl-2-pyrrolicarboxylate methyl N-methylpyrrole-2-carboxylate
Inchi:	InChI=1S/C7H9NO2/c1-8-5-3-4-6(8)7(9)10-2/h3-5H,1-2H3
InchiKey:	APHVGKYWHWFAQV-UHFFFAOYSA-N
Formula:	C7H9NO2
SMILES:	COC(=O)c1cccn1C
Mol. weight [g/mol]:	139.15
CAS:	37619-24-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	0.812		Crippen Method
mcvol	107.450	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	59.20	kJ/mol	298.15	Energetics and molecular structure of alkyl 1-methylpyrrolicarboxylates (alkyl = methyl or ethyl)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37619242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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