

1H-Pyrrole-2-acetic acid, 1-methyl-, methyl ester

Other names:	Methyl 1-methyl-1H-pyrrole-2-acetate Methyl 1-methylpyrrole-2-acetate Methyl 1-methyl-2-pyrroleacetate N-Methylpyrrole-2-acetic acid methyl ester methyl 1-methylpyrrol-2-acetate
Inchi:	InChI=1S/C8H11NO2/c1-9-5-3-4-7(9)6-8(10)11-2/h3-5H,6H2,1-2H3
InchiKey:	CGYVDYLHQYNGFC-UHFFFAOYSA-N
Formula:	C8H11NO2
SMILES:	COC(=O)Cc1cccn1C
Mol. weight [g/mol]:	153.18
CAS:	51856-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	0.741		Crippen Method
mcvol	121.540	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.70	K	0.30	NIST Webbook

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=C51856792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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