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/ci990307l

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