

L-Proline, 1-methyl-, methyl ester

Other names:	Proline, 1-methyl-, methyl ester, L-Methyl (-)-hydrate Methyl 1-methyl-2-pyrrolidinecarboxylate, (L)-Proline, 1-methyl, methyl ester
Inchi:	InChI=1S/C7H13NO2/c1-8-5-3-4-6(8)7(9)10-2/h6H,3-5H2,1-2H3
InchiKey:	WBXUFOSSZLFNPQ-UHFFFAOYSA-N
Formula:	C7H13NO2
SMILES:	COC(=O)C1CCCN1C
Mol. weight [g/mol]:	143.18
CAS:	27957-91-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	0.254		Crippen Method
mcvol	116.050	ml/mol	McGowan Method
rinsol	1017.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C27957911&Units=SI

Legend

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

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