

D-Proline, N-methoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C9H15NO4/c1-3-14-8(11)7-5-4-6-10(7)9(12)13-2/h7H,3-6H2,1-2H3
InchiKey: NWFRFHYYYBQONU-UHFFFAOYSA-N
Formula: C9H15NO4
SMILES: CCOC(=O)C1CCCN1C(=O)OC
Mol. weight [g/mol]: 201.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Cheméo Relay (1.0)
logp	0.780		Crippen Method
mcvol	151.670	ml/mol	McGowan Method
rinpol	1478.00		NIST Webbook
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tb	545.06	K	Cheméo Relay (1.0)
tf	312.65	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320786&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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