

d-Proline, N-ethoxycarbonyl-, isoheptyl ester

Inchi: InChI=1S/C14H25NO4/c1-4-18-14(17)15-9-5-8-12(15)13(16)19-10-6-7-11(2)3/h11-12H,4
InchiKey: WMHGVDRFXWIZLY-UHFFFAOYSA-N
Formula: C14H25NO4
SMILES: CCOC(=O)N1CCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	2.587		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		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=U320836&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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/11-644-4/d-Proline-N-ethoxycarbonyl-isoheptyl-ester.pdf>

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