

d-Proline, N-isobutoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C24H45NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-28-23(26)22-17-16-18-25(2)
InchiKey: ZOWQWHJNPRPPFY-UHFFFAOYSA-N
Formula: C24H45NO4
SMILES: CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 411.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	6.488		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
rinsol	2618.00		NIST Webbook
rinsol	2618.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320813&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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