

d-Proline, N-isobutoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C22H41NO4/c1-4-5-6-7-8-9-10-11-12-13-17-26-21(24)20-15-14-16-23(20)22(20)21-3
InchiKey: XVBXPEISHYKJMB-UHFFFAOYSA-N
Formula: C22H41NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	5.708		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320812&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
rinpol: Non-polar retention indices

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