

# d-Proline, N-isobutoxycarbonyl-, pentadecyl ester

Inchi:	InChI=1S/C25H47NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-29-24(27)23-18-17-19-2
InchiKey:	XFMWCKULNPJPNZ-UHFFFAOYSA-N
Formula:	C25H47NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]:	425.64

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.33		Crippen Method
logp	6.878		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U320814&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320814&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## 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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