

L-Proline, N-(2-bromobenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C26H40BrNO3/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-31-26(30)24-19-16-20-28(2
InchiKey:	IXLDFNERBEMFI-UHFFFAOYSA-N
Formula:	C26H40BrNO3
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]:	494.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.76		Crippen Method
logp	7.298		Crippen Method
mcvol	379.070	ml/mol	McGowan Method
rinpol	3535.00		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=U346230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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