d-Proline, n-butoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C19H35NO4/c1-3-5-7-8-9-10-11-16-23-18(21)17-13-12-14-20(17)19(22)24-15-
InchiKey: COARSCXNGUFDGL-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)OCCCC
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	4.681		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		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=U321087&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

Latest version available from:
https://www.chemeo.com/cid/99-644-8/d-Proline-n-butoxycarbonyl-nonyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:28:49.822376595 +0000 UTC m=+3284592.459345844.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.