

D-Pro, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C16H22N2O3/c1-3-21-16(20)18-11-7-10-14(18)15(19)17-12(2)13-8-5-4-6-9-13
InchiKey: FCMOKSLYERJIEZ-GXTWGEPZSA-N
Formula: C16H22N2O3
SMILES: CCOC(=O)N1CCCC1C(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 290.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.485		Crippen Method
mcvol	230.650	ml/mol	McGowan Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		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=R587523&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/60-479-4/D-Pro-N-ethoxycarbonyl-S-1-phenylethylamide.pdf>

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