

d-Proline, N-allyloxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C13H21NO4/c1-4-8-17-13(16)14-7-5-6-11(14)12(15)18-9-10(2)3/h4,10-11H,1,5,8,12,13,16,17,18H2
InchiKey: LLWRIWUEFYEZFR-UHFFFAOYSA-N
Formula: C13H21NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 255.31

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.16 | | Crippen Method |
| logp | 1.973 | | Crippen Method |
| mcvol | 203.730 | ml/mol | McGowan Method |
| rinpol | 1755.00 | | NIST Webbook |
| rinpol | 1755.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320964&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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