

Pipecolic acid, N-butoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C20H37NO4/c1-3-5-7-8-9-10-13-17-24-19(22)18-14-11-12-15-21(18)20(23)25-
InchiKey: KGQUCYVDNCDKCG-UHFFFAOYSA-N
Formula: C20H37NO4
SMILES: CCCCCCCCCOC(=O)C1CCCCN1C(=O)OCCCC
Mol. weight [g/mol]: 355.51

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.47 | | Crippen Method |
| logp | 5.071 | | Crippen Method |
| mcvol | 306.660 | ml/mol | McGowan Method |
| rinpol | 2446.00 | | NIST Webbook |
| rinpol | 2446.00 | | 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=U393055&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

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