

L-Norvaline, N-hexyloxycarbonyl-, undecyl ester

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|----------------------|---|
| Inchi: | InChI=1S/C23H45NO4/c1-4-7-9-11-12-13-14-15-17-19-27-22(25)21(18-6-3)24-23(26)28 |
| InchiKey: | OPFIJUCHEXLXCW-OAQYLSRUSA-N |
| Formula: | C23H45NO4 |
| SMILES: | CCCCCCCCCCCCOC(=O)C(CCC)N=C(O)OCCCCC |
| Mol. weight [g/mol]: | 399.61 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -980.15 | kJ/mol | Joback Method |
| hvap | 98.04 | kJ/mol | Joback Method |
| log10ws | -6.99 | | Crippen Method |
| logp | 6.740 | | Crippen Method |
| mcvol | 359.790 | ml/mol | McGowan Method |
| pc | 866.58 | kPa | Joback Method |
| rinpol | 2693.00 | | NIST Webbook |
| rinpol | 2693.00 | | NIST Webbook |
| tb | 992.65 | K | Joback Method |
| tc | 1224.98 | K | Joback Method |

Sources

| | |
|-----------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392838&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-------|---|
| hf: | Enthalpy of formation at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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