

L-Norvaline, N-octyloxycarbonyl-, isobutyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C18H35NO4/c1-5-7-8-9-10-11-13-22-18(21)19-16(12-6-2)17(20)23-14-15(3)4/ |
| InchiKey: | ZNANAXDXIXJEOG-MRXNPFEDSA-N |
| Formula: | C18H35NO4 |
| SMILES: | CCCCCCCCOC(O)=NC(CCC)C(=O)OCC(C)C |
| Mol. weight [g/mol]: | 329.47 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -882.23 | kJ/mol | Joback Method |
| hvap | 86.52 | kJ/mol | Joback Method |
| log10ws | -4.66 | | Crippen Method |
| logp | 4.645 | | Crippen Method |
| mcvol | 289.340 | ml/mol | McGowan Method |
| pc | 1181.71 | kPa | Joback Method |
| rinpol | 2157.00 | | NIST Webbook |
| rinpol | 2157.00 | | NIST Webbook |
| tb | 877.81 | K | Joback Method |
| tc | 1075.29 | K | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392843&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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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