

L-Norvaline, N-isobutoxycarbonyl-, hexadecyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C26H51NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-30-25(28)24(20-6 |
| InchiKey: | OFEFFOWEOYMBJC-UHFFFAOYSA-N |
| Formula: | C26H51NO4 |
| SMILES: | CCCCCCCCCCCCCCCCOC(=O)C(CCC)N=C(O)OCC(C)C |
| Mol. weight [g/mol]: | 441.69 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|--------|----------------|
| hf | -1047.35 | kJ/mol | Joback Method |
| hvap | 104.33 | kJ/mol | Joback Method |
| log10ws | -8.00 | | Crippen Method |
| logp | 7.766 | | Crippen Method |
| mcvol | 402.060 | ml/mol | McGowan Method |
| pc | 739.63 | kPa | Joback Method |
| tb | 1060.85 | K | Joback Method |
| tc | 1326.13 | 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=U320724&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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