# DL-3-Aminobutanoic acid, N-(2-ethylhexyl)oxycarbonyl-, dodecyl ester

**Inchi:** InChI=1S/C25H49NO4/c1-5-8-10-11-12-13-14-15-16-17-19-29-24(27)20-22(4)26-25(28)3

**InchiKey:** VFISRKBZQRXFBV-UHFFFAOYSA-N

**Formula:** C25H49NO4

**SMILES:** CCCCCCCCCCCCOC(=O)CC(C)N=C(O)OCC(CC)CCCC

**Mol. weight [g/mol]:** 427.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -1026.71 | kJ/mol | Joback Method |
| hvap | 102.11 | kJ/mol | Joback Method |
| log10ws | -7.59 | | Crippen Method |
| logp | 7.376 | | Crippen Method |
| mcvol | 387.970 | ml/mol | McGowan Method |
| pc | 779.81 | kPa | Joback Method |
| rinpol | 2877.00 | | NIST Webbook |
| rinpol | 2877.00 | | NIST Webbook |
| tb | 1037.97 | K | Joback Method |
| tc | 1290.19 | K | Joback Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**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=U392824&Units=SI

## 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 |