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

**Inchi:** InChI=1S/C20H39NO4/c1-5-8-10-11-12-14-24-19(22)15-17(4)21-20(23)25-16-18(7-3)13-

**InchiKey:** JYHYMOLFZFXDTE-UHFFFAOYSA-N

**Formula:** C20H39NO4

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

**Mol. weight [g/mol]:** 357.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -923.51 | kJ/mol | Joback Method |
| hvap | 90.98 | kJ/mol | Joback Method |
| log10ws | -5.49 | | Crippen Method |
| logp | 5.426 | | Crippen Method |
| mcvol | 317.520 | ml/mol | McGowan Method |
| pc | 1039.91 | kPa | Joback Method |
| rinpol | 2399.00 | | NIST Webbook |
| rinpol | 2399.00 | | NIST Webbook |
| tb | 923.57 | K | Joback Method |
| tc | 1131.08 | K | Joback Method |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U392820&Units=SI

**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

## 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 |