# 2-Aminopent-4-enoic acid, N-(2-ethylhexyloxycarbonyl)-, 2-ethylhexyl ester

**Inchi:** InChI=1S/C22H41NO4/c1-6-11-14-18(9-4)16-26-21(24)20(13-8-3)23-22(25)27-17-19(10-

**InchiKey:** BRNMVQGNMCWOAX-UHFFFAOYSA-N

**Formula:** C22H41NO4

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

**Mol. weight [g/mol]:** 383.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -844.64 | kJ/mol | Joback Method |
| hvap | 94.37 | kJ/mol | Joback Method |
| log10ws | -5.94 | | Crippen Method |
| logp | 5.838 | | Crippen Method |
| mcvol | 341.400 | ml/mol | McGowan Method |
| pc | 950.84 | kPa | Joback Method |
| rinpol | 2363.00 | | NIST Webbook |
| rinpol | 2363.00 | | NIST Webbook |
| tb | 965.57 | K | Joback Method |
| tc | 1184.23 | 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=U393170&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 |