# «beta»-Alanine, N-(3-methylbut-2-enoyl)-, dodecyl ester

**Inchi:** InChI=1S/C20H37NO3/c1-4-5-6-7-8-9-10-11-12-13-16-24-20(23)14-15-21-19(22)17-18(2

**InchiKey:** VTDIKYPZGKKGBZ-UHFFFAOYSA-N

**Formula:** C20H37NO3

**SMILES:** CCCCCCCCCCCCOC(=O)CCN=C(O)C=C(C)C

**Mol. weight [g/mol]:** 339.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -673.30 | kJ/mol | Joback Method |
| hvap | 89.38 | kJ/mol | Joback Method |
| log10ws | -5.89 | | Crippen Method |
| logp | 5.763 | | Crippen Method |
| mcvol | 307.350 | ml/mol | McGowan Method |
| pc | 1079.93 | kPa | Joback Method |
| rinpol | 2587.00 | | NIST Webbook |
| tb | 906.07 | K | Joback Method |
| tc | 1109.30 | 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=U321955&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |