

2-Aminopent-4-enoic acid, N-hexyloxycarbonyl-, tridecyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C25H47NO4/c1-4-7-9-11-12-13-14-15-16-17-19-21-29-24(27)23(20-6-3)26-25 |
| InchiKey: | DOSUVENEDQDXKC-UHFFFAOYSA-N |
| Formula: | C25H47NO4 |
| SMILES: | C=CCC(N=C(O)OCCCCC)C(=O)OCCCCCCCCCCCC |
| Mol. weight [g/mol]: | 425.64 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -896.00 | kJ/mol | Joback Method |
| hvap | 101.82 | kJ/mol | Joback Method |
| log10ws | -7.68 | | Crippen Method |
| logp | 7.296 | | Crippen Method |
| mcvol | 383.670 | ml/mol | McGowan Method |
| pc | 794.84 | kPa | Joback Method |
| rinpol | 2828.00 | | NIST Webbook |
| rinpol | 2828.00 | | NIST Webbook |
| tb | 1035.09 | K | Joback Method |
| tc | 1286.09 | 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=U393146&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |

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