

L-Norvaline, N-octyloxycarbonyl-, nonyl ester

Inchi: InChI=1S/C23H45NO4/c1-4-7-9-11-13-15-16-19-27-22(25)21(18-6-3)24-23(26)28-20-17-12-5-8-10-14-17-20-22-23-25-26-28-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: PMZYJXBROAPQKV-OAQYLSRUSA-N
Formula: C23H45NO4
SMILES: CCCCCCCCCOC(=O)C(CCC)N=C(O)OCCCCCCCC
Mol. weight [g/mol]: 399.61

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -980.15 | kJ/mol | Joback Method |
| hvap | 98.04 | kJ/mol | Joback Method |
| log10ws | -6.99 | | Crippen Method |
| logp | 6.740 | | Crippen Method |
| mcvol | 359.790 | ml/mol | McGowan Method |
| pc | 866.58 | kPa | Joback Method |
| rinpol | 2686.00 | | NIST Webbook |
| rinpol | 2686.00 | | NIST Webbook |
| tb | 992.65 | K | Joback Method |
| tc | 1224.98 | 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=U392849&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 |

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