

# Glycine, 2-cyclohexyl-N-methoxycarbonyl-, nonyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C19H35NO4/c1-3-4-5-6-7-8-12-15-24-18(21)17(20-19(22)23-2)16-13-10-9-11- |
| InchiKey:            | JXNUZLUNGHKWQH-UHFFFAOYSA-N  |
| Formula:             | C19H35NO4  |
| SMILES:              | CCCCCCCCCCOC(=O)C(N=C(O)OC)C1CCCCC1  |
| Mol. weight [g/mol]: | 341.49   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -843.27 | kJ/mol | Joback Method  |
| hvap          | 89.57   | kJ/mol | Joback Method  |
| log10ws       | -4.97   |        | Crippen Method |
| logp          | 4.790   |        | Crippen Method |
| mcvol         | 292.570 | ml/mol | McGowan Method |
| pc            | 1268.25 | kPa    | Joback Method  |
| rinpol        | 2378.00 |        | NIST Webbook   |
| rinpol        | 2378.00 |        | NIST Webbook   |
| tb            | 920.68  | K      | Joback Method  |
| tc            | 1129.56 | K      | Joback Method  |

## Sources

|                 |   |
|-----------------|---|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U383095&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383095&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|       |   |
|-------|---|
| hf:   | Enthalpy of formation at standard conditions    |
| hvap: | Enthalpy of vaporization at standard conditions |

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>pc:</b>      | Critical Pressure                   |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |

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