

«gamma»-Aminobutyric acid, N-isobutoxycarbonyl-, nonyl ester

Other names: .gama.-Aminobutyric acid, N-isobutoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C18H35NO4/c1-4-5-6-7-8-9-10-14-22-17(20)12-11-13-19-18(21)23-15-16(2)3/

InchiKey: OCNVQVKIPHJQPY-UHFFFAOYSA-N

Formula: C18H35NO4

SMILES: CCCCCCCCCOC(=O)CCCN=C(O)OCC(C)C

Mol. weight [g/mol]: 329.47

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -876.95 | kJ/mol | Joback Method |
| hvap | 86.91 | kJ/mol | Joback Method |
| log10ws | -4.54 | | Crippen Method |
| logp | 4.647 | | Crippen Method |
| mcvol | 289.340 | ml/mol | McGowan Method |
| pc | 1175.24 | kPa | Joback Method |
| tb | 878.25 | K | Joback Method |
| tc | 1075.49 | 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=U321052&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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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