

O-nitro carbanilic acid, l-menthyl ester

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| Inchi: | InChI=1S/C17H24N2O4/c1-11(2)13-9-8-12(3)16(10-13)23-17(20)18-14-6-4-5-7-15(14)19 |
| InchiKey: | GVUNJXKRYBHIQK-UHFFFAOYSA-N |
| Formula: | C17H24N2O4 |
| SMILES: | CC(C)C1CCC(C)C(OC(=O)Nc2ccccc2[N+](=O)[O-])C1 |
| Mol. weight [g/mol]: | 320.38 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 92.65 | kJ/mol | Joback Method |
| hf | -362.88 | kJ/mol | Joback Method |
| hfus | 43.14 | kJ/mol | Joback Method |
| hvap | 87.98 | kJ/mol | Joback Method |
| log10ws | -5.44 | | Crippen Method |
| logp | 4.604 | | Crippen Method |
| mcvol | 250.610 | ml/mol | McGowan Method |
| pc | 1864.33 | kPa | Joback Method |
| tb | 908.09 | K | Joback Method |
| tc | 1151.45 | K | Joback Method |
| tf | 572.62 | K | Joback Method |
| vc | 0.946 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 832.41 | J/molxK | 908.09 | Joback Method |
| cpg | 847.60 | J/molxK | 948.65 | Joback Method |
| cpg | 861.08 | J/molxK | 989.21 | Joback Method |
| cpg | 872.89 | J/molxK | 1029.77 | Joback Method |
| cpg | 883.08 | J/molxK | 1070.33 | Joback Method |
| cpg | 891.68 | J/molxK | 1110.89 | Joback Method |
| cpg | 898.76 | J/molxK | 1151.45 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=B6002464&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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