

Glutaric acid, ethyl 2-(4-nitrophenoxy)ethyl ester

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| Inchi: | InChI=1S/C15H19NO7/c1-2-21-14(17)4-3-5-15(18)23-11-10-22-13-8-6-12(7-9-13)16(19) |
| InchiKey: | MJXUKNBDJWQVPN-UHFFFAOYSA-N |
| Formula: | C15H19NO7 |
| SMILES: | CCOC(=O)CCCC(=O)OCCOc1ccc([N+](=O)[O-])cc1 |
| Mol. weight [g/mol]: | 325.31 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -359.09 | kJ/mol | Joback Method |
| hf | -760.45 | kJ/mol | Joback Method |
| hfus | 46.38 | kJ/mol | Joback Method |
| hvap | 89.23 | kJ/mol | Joback Method |
| log10ws | -3.32 | | Crippen Method |
| logp | 2.250 | | Crippen Method |
| mcvol | 236.620 | ml/mol | McGowan Method |
| pc | 1966.56 | kPa | Joback Method |
| rinqol | 2608.00 | | NIST Webbook |
| tb | 901.10 | K | Joback Method |
| tc | 1124.19 | K | Joback Method |
| tf | 607.91 | K | Joback Method |
| vc | 0.915 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 724.14 | J/molxK | 901.10 | Joback Method |
| cpg | 735.42 | J/molxK | 938.28 | Joback Method |
| cpg | 745.45 | J/molxK | 975.46 | Joback Method |
| cpg | 754.25 | J/molxK | 1012.65 | Joback Method |
| cpg | 761.80 | J/molxK | 1049.83 | Joback Method |
| cpg | 768.11 | J/molxK | 1087.01 | Joback Method |
| cpg | 773.19 | J/molxK | 1124.19 | 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=U376792&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| 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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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