

Glycolic acid, nitrate, isobutyl ester

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| Inchi: | InChI=1S/C6H11NO5/c1-5(2)3-11-6(8)4-12-7(9)10/h5H,3-4H2,1-2H3 |
| InchiKey: | CKQILHWPHTJBO-UHFFFAOYSA-N |
| Formula: | C6H11NO5 |
| SMILES: | CC(C)COC(=O)CO[N+](=O)[O-] |
| Mol. weight [g/mol]: | 177.16 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -306.17 | kJ/mol | Joback Method |
| hf | -560.23 | kJ/mol | Joback Method |
| hfus | 23.11 | kJ/mol | Joback Method |
| hvap | 56.72 | kJ/mol | Joback Method |
| log10ws | -1.12 | | Crippen Method |
| logp | 0.394 | | Crippen Method |
| mcvol | 126.130 | ml/mol | McGowan Method |
| pc | 3284.05 | kPa | Joback Method |
| tb | 586.79 | K | Joback Method |
| tc | 797.60 | K | Joback Method |
| tf | 380.38 | K | Joback Method |
| vc | 0.489 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 310.17 | J/molxK | 586.79 | Joback Method |
| cpg | 321.01 | J/molxK | 621.92 | Joback Method |
| cpg | 331.31 | J/molxK | 657.06 | Joback Method |
| cpg | 341.06 | J/molxK | 692.19 | Joback Method |
| cpg | 350.26 | J/molxK | 727.33 | Joback Method |
| cpg | 358.89 | J/molxK | 762.46 | Joback Method |
| cpg | 366.95 | J/molxK | 797.60 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R633042&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| 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 |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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