

Acetic acid, [(benzoylamino)oxy]-

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|-----------------------------|---|
| Other names: | Benzadox Acetic acid, (benzamidoxy)- Benzamidoxyacetic acid Benzamidoxyacetic acid Hydroxylamine, N-benzoyl-O-(carboxymethyl)- S 6173 o-Benzamidoglycolic acid ((Benzoylamino)oxy)acetic acid S-7,173 S-7173 Topcide Topicide NSC 75601 |
| Inchi: | InChI=1S/C9H9NO4/c11-8(12)6-14-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12) |
| InchiKey: | WDRGQGLIUAMOOO-UHFFFAOYSA-N |
| Formula: | C9H9NO4 |
| SMILES: | O=C(O)CONC(=O)c1ccccc1 |
| Mol. weight [g/mol]: | 195.17 |
| CAS: | 5251-93-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|---------|----------------|
| gf | -272.96 | kJ/mol | Joback Method |
| hf | -448.70 | kJ/mol | Joback Method |
| hfus | 26.68 | kJ/mol | Joback Method |
| hvap | 76.92 | kJ/mol | Joback Method |
| log10ws | -1.41 | | Crippen Method |
| logp | 0.433 | | Crippen Method |
| mcvol | 138.770 | ml/mol | McGowan Method |
| pc | 4233.04 | kPa | Joback Method |
| tb | 704.51 | K | Joback Method |
| tc | 912.69 | K | Joback Method |
| tf | 417.66 ± 0.20 | K | NIST Webbook |
| tf | 417.60 ± 0.20 | K | NIST Webbook |
| vc | 0.515 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 360.04 | J/mol×K | 704.51 | Joback Method |
| cpg | 369.10 | J/mol×K | 739.21 | Joback Method |
| cpg | 377.50 | J/mol×K | 773.90 | Joback Method |
| cpg | 385.26 | J/mol×K | 808.60 | Joback Method |
| cpg | 392.38 | J/mol×K | 843.30 | Joback Method |
| cpg | 398.90 | J/mol×K | 877.99 | Joback Method |
| cpg | 404.82 | J/mol×K | 912.69 | Joback Method |
| hfust | 31.46 | kJ/mol | 416.90 | NIST Webbook |
| hfust | 31.46 | kJ/mol | 416.90 | NIST Webbook |

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=C5251934&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| hfust: | Enthalpy of fusion at a given temperature |
| 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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