

3,4,5-Trimethoxybenzhydrazide

Other names:

3,4,5-Trimethoxybenzoic acid hydrazide
3,4,5-Trimethoxybenzoic hydrazide
Benzoic acid, 3,4,5-trimethoxy-, hydrazide
Benzhydrazide, 3,4,5-trimethoxy-
Benzohydrazide, 3,4,5-trimethoxy-
3,4,5-trimethoxybenzohydrazide

Inchi: InChI=1S/C10H14N2O4/c1-14-7-4-6(10(13)12-11)5-8(15-2)9(7)16-3/h4-5H,11H2,1-3H3,**InchiKey:** KQXHMNUXNHQSOW-UHFFFAOYSA-N**Formula:** C10H14N2O4**SMILES:** COc1cc(C(=O)NN)cc(OC)c1OC**Mol. weight [g/mol]:** 226.23**CAS:** 3291-03-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -171.24 | kJ/mol | Joback Method |
| hf | -469.59 | kJ/mol | Joback Method |
| hfus | 29.99 | kJ/mol | Joback Method |
| hvap | 73.17 | kJ/mol | Joback Method |
| log10ws | -2.18 | | Crippen Method |
| logp | 0.316 | | Crippen Method |
| mcvol | 167.140 | ml/mol | McGowan Method |
| pc | 3052.41 | kPa | Joback Method |
| tb | 713.65 | K | Joback Method |
| tc | 931.11 | K | Joback Method |
| tf | 518.98 | K | Joback Method |
| vc | 0.612 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 452.17 | J/mol×K | 713.65 | Joback Method |
| cpg | 464.29 | J/mol×K | 749.89 | Joback Method |
| cpg | 475.62 | J/mol×K | 786.14 | Joback Method |

| | | | | |
|-----|--------|---------|--------|---------------|
| cpg | 486.13 | J/mol×K | 822.38 | Joback Method |
| cpg | 495.80 | J/mol×K | 858.62 | Joback Method |
| cpg | 504.60 | J/mol×K | 894.87 | Joback Method |
| cpg | 512.51 | J/mol×K | 931.11 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3291030&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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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