

2,2,2-Trichloro-n'-(4-chlorobenzoyl)acetohydrazid

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|-----------------------------|---|
| Inchi: | InChI=1S/C9H6Cl4N2O2/c10-6-3-1-5(2-4-6)7(16)14-15-8(17)9(11,12)13/h1-4H,(H,14,16) |
| InchiKey: | JQIUHCMAAQLMOY-UHFFFAOYSA-N |
| Formula: | C9H6Cl4N2O2 |
| SMILES: | O=C(NNC(=O)C(Cl)(Cl)Cl)c1ccc(Cl)cc1 |
| Mol. weight [g/mol]: | 315.97 |
| CAS: | 64968-99-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 3.74 | kJ/mol | Joback Method |
| hf | -193.96 | kJ/mol | Joback Method |
| hfus | 35.49 | kJ/mol | Joback Method |
| hvap | 81.17 | kJ/mol | Joback Method |
| log10ws | -4.44 | | Crippen Method |
| logp | 2.471 | | Crippen Method |
| mcvol | 185.970 | ml/mol | McGowan Method |
| pc | 3291.59 | kPa | Joback Method |
| tb | 791.55 | K | Joback Method |
| tc | 1040.90 | K | Joback Method |
| tf | 557.41 | K | Joback Method |
| vc | 0.699 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 419.33 | J/molxK | 791.55 | Joback Method |
| cpg | 426.51 | J/molxK | 833.11 | Joback Method |
| cpg | 432.92 | J/molxK | 874.67 | Joback Method |
| cpg | 438.64 | J/molxK | 916.23 | Joback Method |
| cpg | 443.77 | J/molxK | 957.78 | Joback Method |
| cpg | 448.38 | J/molxK | 999.34 | Joback Method |
| cpg | 452.57 | J/molxK | 1040.90 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=C64968996&Units=SI |

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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