

Carbamothioic acid, S-[2-oxo-2-(phenylamino)ethyl] ester

Other names:

Acetamide, N-phenyl-2-(carbamoylthio)-
Acetanilide, 2-(thiocarbamyl)-
Carbamic acid, thio-, S-ester with 2-mercaptopropanilide
Carbaminothioglycolic acid anilide
NSC 13336
S-[2-oxo-2-(phenylamino)ethyl] aminomethanethioate
USAF uctl-1766
alpha-Mercaptoacetanilide carbamate
«alpha»-(Thiocarbamyl) acetanilide
Â«alphaÂ»-(Thiocarbamyl) acetanilide

Inchi: InChI=1S/C9H10N2O2S/c10-9(13)14-6-8(12)11-7-4-2-1-3-5-7/h1-5H,6H2,(H2,10,13)(H,14)
InchiKey: CEINNGQDMFZTJK-UHFFFAOYSA-N
Formula: C9H10N2O2S
SMILES: NC(=O)SCC(=O)Nc1ccccc1
Mol. weight [g/mol]: 210.25
CAS: 5428-95-5

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|--------------------------------------|
| gf | 68.43 | kJ/mol | Joback Method |
| hf | -88.59 | kJ/mol | Joback Method |
| hfus | 30.73 | kJ/mol | Joback Method |
| hvap | 75.29 | kJ/mol | Joback Method |
| log10ws | -1.32 | | Aqueous Solubility Prediction Method |
| logp | 1.437 | | Crippen Method |
| mcvol | 153.360 | ml/mol | McGowan Method |
| pc | 4227.54 | kPa | Joback Method |
| tb | 731.22 | K | Joback Method |
| tc | 980.54 | K | Joback Method |
| tf | 487.79 | K | Joback Method |
| vc | 0.561 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 391.18 | J/mol×K | 731.22 | Joback Method |
| cpg | 401.66 | J/mol×K | 772.77 | Joback Method |
| cpg | 411.16 | J/mol×K | 814.33 | Joback Method |
| cpg | 419.70 | J/mol×K | 855.88 | Joback Method |
| cpg | 427.35 | J/mol×K | 897.43 | Joback Method |
| cpg | 434.13 | J/mol×K | 938.99 | Joback Method |
| cpg | 440.09 | J/mol×K | 980.54 | Joback Method |

Sources

- Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>
- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5428955&Units=SI>
- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- 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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