

Ethylthiocarbamic acid, 2-formylhydrazide

Inchi: InChI=1S/C4H9N3OS/c1-2-5-4(9)7-6-3-8/h3H,2H2,1H3,(H,6,8)(H2,5,7,9)
InchiKey: BLJFHNQORZOJQD-UHFFFAOYSA-N
Formula: C4H9N3OS
SMILES: CCN=C(S)NN=CO
Mol. weight [g/mol]: 147.20
CAS: 31409-15-1

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -31.52 | kJ/mol | Joback Method |
| hvap | 61.06 | kJ/mol | Joback Method |
| log10ws | -0.89 | | Crippen Method |
| logp | 0.383 | | Crippen Method |
| mcvol | 110.780 | ml/mol | McGowan Method |
| pc | 3727.11 | kPa | Joback Method |
| tb | 649.37 | K | Joback Method |
| tc | 871.16 | K | Joback Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C31409151&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation 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 |

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