

# Hydrazinecarbothioamide, N-ethyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Semicarbazide, 4-ethyl-3-thio-<br>B 1131<br>Ethylthiosemicarbazide<br>4-Ethyl-3-Thiosemicarbazide<br>4-Ethylthiosemicarbazide<br>Thiosemicarbazide, 4-ethyl- |
| <b>Inchi:</b>               | InChI=1S/C3H9N3S/c1-2-5-3(7)6-4/h2,4H2,1H3,(H2,5,6,7)  |
| <b>InchiKey:</b>            | SKYYTGUCWARUCL-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C3H9N3S  |
| <b>SMILES:</b>              | CCN=C(S)NN   |
| <b>Mol. weight [g/mol]:</b> | 119.19   |
| <b>CAS:</b>                 | 13431-34-0   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | 92.92   | kJ/mol | Joback Method  |
| hvap          | 49.48   | kJ/mol | Joback Method  |
| log10ws       | -0.92   |        | Crippen Method |
| logp          | -0.245  |        | Crippen Method |
| mcvol         | 95.120  | ml/mol | McGowan Method |
| pc            | 4615.13 | kPa    | Joback Method  |
| tb            | 530.16  | K      | Joback Method  |
| tc            | 767.79  | K      | Joback Method  |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>   |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13431340&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13431340&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |

# Legend

|                            |   |
|----------------------------|---|
| <b>hf:</b>                 | Enthalpy of formation at standard conditions    |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log10 of Water solubility in mol/l              |
| <b>log<sub>p</sub>:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>              | McGowan's characteristic volume                 |
| <b>pc:</b>                 | Critical Pressure                               |
| <b>tb:</b>                 | Normal Boiling Point Temperature                |
| <b>tc:</b>                 | Critical Temperature                            |

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