

Ethane, isocyanato-

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|-----------------------------|---|
| Other names: | C2H5NCO Ethyl isocyanate Isocyanatoethane Isocyanic acid, ethyl ester UN 2481 |
| Inchi: | InChI=1S/C3H5NO/c1-2-4-3-5/h2H2,1H3 |
| InchiKey: | WUDNUHPRLBTKOJ-UHFFFAOYSA-N |
| Formula: | C3H5NO |
| SMILES: | CCN=C=O |
| Mol. weight [g/mol]: | 71.08 |
| CAS: | 109-90-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------------|--------|----------------|
| hf | -110.66 | kJ/mol | Joback Method |
| hvap | 31.80 | kJ/mol | Joback Method |
| ie | 10.10 | eV | NIST Webbook |
| ie | 10.32 ± 0.05 | eV | NIST Webbook |
| log10ws | -4.58 | | Crippen Method |
| logp | 0.342 | | Crippen Method |
| mcvol | 60.380 | ml/mol | McGowan Method |
| pc | 4876.56 | kPa | Joback Method |
| tb | 334.71 | K | Joback Method |
| tc | 514.09 | K | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.52808e+01 |
| Coeff. B | -3.23484e+03 |
| Coeff. C | -3.37660e+01 |
| Temperature range (K), min. | 249.52 |

Sources

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|---|---|
| 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=C109900&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| hf: | Enthalpy of formation at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pvap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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