

Lethane

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| Other names: | Thiocyanic acid, 2-(2-butoxyethoxy)ethyl ester Butyl carbitol rhodanate Lethane 384 1-Butoxy-2-(2-thiocyanoethoxy)ethane 2-(2-Butoxyethoxy)ethyl thiocyanate «beta»-Butoxy-«beta»'-thiocyanodiethyl ether Butoxyrhodanodiethyl ether Butyl carbitol thiocyanate Ethane, 1-butoxy-2-(2-thiocyanatoethoxy)- Ethanol, 2-(2-butoxyethoxy)-, thiocyanate ENT 6 2-(2-(Butoxy)ethoxy)ethyl thiocyanic acid ester 2-Butoxy-2'-thiocyanodiethyl ether 2-(2-Butoxyethoxy)ethylthiokyanat 1-Butoxy-«alpha»-(2-thiocyanoethoxy)ethane Lethane 384 regular NSC 3534 |
| Inchi: | InChI=1S/C9H17NO2S/c1-2-3-4-11-5-6-12-7-8-13-9-10/h2-8H2,1H3 |
| InchiKey: | JVGPVVUTUMQJKL-UHFFFAOYSA-N |
| Formula: | C9H17NO2S |
| SMILES: | CCCCOCCOCCSC#N |
| Mol. weight [g/mol]: | 203.30 |
| CAS: | 112-56-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -18.80 | kJ/mol | Joback Method |
| hf | -286.78 | kJ/mol | Joback Method |
| hfus | 27.08 | kJ/mol | Joback Method |
| hvap | 57.74 | kJ/mol | Joback Method |
| log10ws | -2.01 | | Crippen Method |
| logp | 2.034 | | Crippen Method |
| mcvol | 167.140 | ml/mol | McGowan Method |
| pc | 2216.62 | kPa | Joback Method |
| tb | 621.02 | K | Joback Method |
| tc | 818.50 | K | Joback Method |
| tf | 335.04 | K | Joback Method |

vc

0.655

m³/kmol

Joback Method

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 415.21 | J/mol×K | 621.02 | Joback Method |
| cpg | 427.84 | J/mol×K | 653.93 | Joback Method |
| cpg | 439.88 | J/mol×K | 686.85 | Joback Method |
| cpg | 451.34 | J/mol×K | 719.76 | Joback Method |
| cpg | 462.21 | J/mol×K | 752.68 | Joback Method |
| cpg | 472.46 | J/mol×K | 785.59 | Joback Method |
| cpg | 482.10 | J/mol×K | 818.50 | Joback Method |

Sources

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=C112561&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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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