

1-Nonadecanethiol

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C19H40S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20/h20H,2-19H2 |
| InchiKey: | YNESSCJHABBEIO-UHFFFAOYSA-N |
| Formula: | C19H40S |
| SMILES: | CCCCCCCCCCCCCCCCCS |
| Mol. weight [g/mol]: | 300.59 |
| CAS: | 53193-23-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 138.49 | kJ/mol | Joback Method |
| hf | -397.01 | kJ/mol | Joback Method |
| hfus | 49.01 | kJ/mol | Joback Method |
| hvap | 64.62 | kJ/mol | Joback Method |
| log10ws | -7.85 | | Crippen Method |
| logp | 7.568 | | Crippen Method |
| mcvol | 294.920 | ml/mol | McGowan Method |
| pc | 1127.59 | kPa | Joback Method |
| tb | 696.98 | K | Joback Method |
| tc | 869.97 | K | Joback Method |
| tf | 340.35 | K | Joback Method |
| vc | 1.153 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 853.48 | J/molxK | 696.98 | Joback Method |
| cpg | 873.73 | J/molxK | 725.81 | Joback Method |
| cpg | 893.06 | J/molxK | 754.64 | Joback Method |
| cpg | 911.51 | J/molxK | 783.47 | Joback Method |
| cpg | 929.10 | J/molxK | 812.31 | Joback Method |
| cpg | 945.87 | J/molxK | 841.14 | Joback Method |
| cpg | 961.84 | J/molxK | 869.97 | Joback Method |
| hvapt | 79.20 | kJ/mol | 592.00 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.55906e+01 |
| Coeff. B | -5.75429e+03 |
| Coeff. C | -1.20504e+02 |
| Temperature range (K), min. | 496.53 |
| Temperature range (K), max. | 680.31 |

Sources

| | |
|---------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 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 |
| 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=C53193230&Units=SI |

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 |
| hvac: | Enthalpy of vaporization at standard conditions |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pvap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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