# Ethanethiol, 2-(1-adamantyl)amino-, hydrogen sulfate

**Other names:** 2-(1-Adamantyl)aminoethanethiol hydrogen sulfate
S-2-[1-Adamantylamino]ethyl thiosulfuric acid
2-(Adamantylamino)ethanethiol, S-hydrogen sulfate

**Inchi:** InChI=1S/C12H21NO3S2/c14-18(15,16)17-2-1-13-12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11

**InchiKey:** YXDYLGVKBVJRMA-UHFFFAOYSA-N

**Formula:** C12H21NO3S2

**SMILES:** O=S(=O)(O)SCCNC12CC3CC(CC(C3)C1)C2

**Mol. weight [g/mol]:** 291.43

**CAS:** 37018-31-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -275.74 | kJ/mol | Joback Method |
| hf | -594.11 | kJ/mol | Joback Method |
| hfus | 38.61 | kJ/mol | Joback Method |
| hvap | 89.32 | kJ/mol | Joback Method |
| log10ws | -3.13 | | Crippen Method |
| logp | 2.081 | | Crippen Method |
| mcvol | 207.650 | ml/mol | McGowan Method |
| pc | 3602.88 | kPa | Joback Method |
| tb | 752.93 | K | Joback Method |
| tc | 963.44 | K | Joback Method |
| tf | 481.40 | K | Joback Method |
| vc | 0.801 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 643.22 | J/mol×K | 752.93 | Joback Method |
| cpg | 658.92 | J/mol×K | 788.02 | Joback Method |
| cpg | 673.94 | J/mol×K | 823.10 | Joback Method |
| cpg | 688.42 | J/mol×K | 858.19 | Joback Method |
| cpg | 702.54 | J/mol×K | 893.27 | Joback Method |
| cpg | 716.44 | J/mol×K | 928.36 | Joback Method |

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|---|---|---|---|---|
| cpg | 730.27 | J/mol×K | 963.44 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C37018318&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **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 |