

Hexane, 1-(ethylthio)-

Other names: 1-(Ethylsulfanyl)hexane; 3-Thianonane; Ethyl hexyl sulfide; Hexyl ethyl sulfide; Sulfide, ethyl hexyl.

InChI: InChI=1S/C8H18S/c1-3-5-6-7-8-9-4-2/h3-8H2,1-2H3

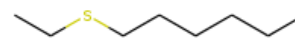
InChI Key: MGUVJBCOCITTRS-UHFFFAOYSA-N

Formula: C8H18S

SMILES: CCCCCSCC

Molecular Weight: 146.29

CAS: 7309-44-6



Physical Properties

| Property | Value | Unit | Source |
|---------------------------------|---------|------------------------|----------------|
| $\Delta_f G^\circ$ | 49.60 | kJ/mol | Joback Method |
| $\Delta_f H^\circ_{\text{gas}}$ | -166.58 | kJ/mol | Joback Method |
| $\Delta_{\text{fus}} H^\circ$ | 20.61 | kJ/mol | Joback Method |
| $\Delta_{\text{vap}} H^\circ$ | 40.22 | kJ/mol | Joback Method |
| $\log P_{\text{oct/wat}}$ | 3.32 | | Crippen Method |
| P_c | 2579.34 | kPa | Joback Method |
| T_{boil} | 451.22 | K | Joback Method |
| T_c | 636.81 | K | Joback Method |
| T_{fus} | 214.32 | K | Joback Method |
| V_c | 0.54 | m ³ /kg-mol | Joback Method |

Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|--------------------|--------|---------|-----------------|---------------|
| $C_{p,\text{gas}}$ | 286.95 | J/mol×K | 451.22 | Joback Method |

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: <http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H18S/c1-3-5-6-7-8-9-4-2/h3-8H2,1-2H3>

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

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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