Dodecane, 1-(ethylthio)-

Other names: Ethyl lauryl sulfide; Sulfide, dodecyl ethyl.
InChI: InChI=1S/C14H30S/c1-3-5-6-7-8-9-10-11-12-13-14-15-4-2/h3-14H2,1-2H3
InChI Key: QECBTJWQRXCSCU-UHFFFAOYSA-N
Formula: C14H30S
SMILES: CCCCCCCCCCCCSCC
Molecular Weight: 230.45
CAS: 2851-83-4

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	100.12	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-290.42	kJ/mol	Joback Method
$\Delta_{fus} H°$	36.15	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.58	kJ/mol	Joback Method
$log P_{oct/wat}$	5.66		Crippen Method
P_c	1543.92	kPa	Joback Method
T_{boil}	588.50	K	Joback Method
T_c	763.97	K	Joback Method
T_{fus}	281.94	K	Joback Method
V_c	0.87	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	575.87	J/mol×K	588.5	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H30S/c1-3-5-6-7-8-9-10-11-12-13-14-15-4-2/h3-14H2,1-2H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).