Ethanamine, 2-(ethylthio)-

Other names: 2-[Ethylthio]ethylamonium
2-(Ethylthio)ethanamine
Inchi: InChI=1S/C4H11NS/c1-2-6-4-3-5/h2-5H2,1H3
InchiKey: HJCTVUWPHAZTLI-UHFFFAOYSA-N
Formula: C4H11NS
SMILES: CCSCCN
Mol. weight [g/mol]: 105.21

Physical Properties

Property code	Value	Unit	Source
hf	-73.18	kJ/mol	Cheméo Relay (1.0)
hfus	15.44	kJ/mol	Joback Method
hvap	47.35	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-0.10		Cheméo Relay (1.0)
logp	0.698		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	438.72	K	Cheméo Relay (1.0)
tc	641.28	K	Cheméo Relay (1.0)
tf	213.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.37	J/mol×K	432.23	Joback Method
cpg	189.87	J/mol×K	466.79	Joback Method
cpg	198.97	J/mol×K	501.35	Joback Method
cpg	207.67	J/mol×K	535.90	Joback Method
cpg	215.98	J/mol×K	570.46	Joback Method
cpg	223.89	J/mol×K	605.02	Joback Method
cpg	231.42	J/mol×K	639.58	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36489039&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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