1-Ethylthio-3-buten-1-yne

Inchi: InChI=1S/C6H8S/c1-3-5-6-7-4-2/h3H,1,4H2,2H3
InchiKey: SICACCNECSLXMB-UHFFFAOYSA-N
Formula: C6H8S
SMILES: C=CC#CSCC
Mol. weight [g/mol]: 112.19
CAS: 14272-36-7

Physical Properties

Property code	Value	Unit	Source
gf	323.40	kJ/mol	Joback Method
hf	272.43	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	37.25	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.886		Crippen Method
mcvol	98.850	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	411.14	K	Joback Method
tc	633.30	K	Joback Method
tf	296.12	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.77	J/mol×K	411.14	Joback Method
cpg	173.97	J/mol×K	448.17	Joback Method
cpg	182.75	J/mol×K	485.19	Joback Method
cpg	191.11	J/mol×K	522.22	Joback Method
cpg	199.07	J/mol×K	559.25	Joback Method
cpg	206.63	J/mol×K	596.28	Joback Method
cpg	213.81	J/mol×K	633.30	Joback Method

Sources

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=C14272367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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