1-Methylthio-3-buten-1-yne

Inchi: InChI=1S/C5H6S/c1-3-4-5-6-2/h3H,1H2,2H3
InchiKey: HIWIEVWZTYIZRX-UHFFFAOYSA-N
Formula: C5H6S
SMILES: C=CC#CSC
Mol. weight [g/mol]: 98.17
CAS: 13030-50-7

Physical Properties

Property code	Value	Unit	Source
gf	314.98	kJ/mol	Joback Method
hf	293.07	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	35.02	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.496		Crippen Method
mcvol	84.760	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	388.26	K	Joback Method
tc	613.01	K	Joback Method
tf	284.85	K	Joback Method
vc	0.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.39	J/mol×K	388.26	Joback Method
cpg	137.85	J/mol×K	425.72	Joback Method
cpg	144.97	J/mol×K	463.18	Joback Method
cpg	151.77	J/mol×K	500.64	Joback Method
cpg	158.26	J/mol×K	538.09	Joback Method
cpg	164.43	J/mol×K	575.55	Joback Method
cpg	170.29	J/mol×K	613.01	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=C13030507&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