

4-Methylthio-3-buten-1-yne

Inchi:	InChI=1S/C5H6S/c1-3-4-5-6-2/h1,4-5H,2H3/b5-4+
InchiKey:	NKMNGGDPEPZMPK-SNAWJCMRSA-N
Formula:	C5H6S
SMILES:	C#CC=CSC
Mol. weight [g/mol]:	98.17
CAS:	3448-56-4

Physical Properties

Property code	Value	Unit	Source
gf	327.63	kJ/mol	Joback Method
hf	304.46	kJ/mol	Joback Method
hfus	16.01	kJ/mol	Joback Method
hvap	33.36	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.496		Crippen Method
mcvol	84.760	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	376.86	K	Joback Method
tc	593.17	K	Joback Method
tf	222.40	K	Joback Method
vc	0.311	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.79	J/mol×K	376.86	Joback Method
cpg	139.45	J/mol×K	412.91	Joback Method
cpg	146.65	J/mol×K	448.96	Joback Method
cpg	153.39	J/mol×K	485.02	Joback Method
cpg	159.72	J/mol×K	521.07	Joback Method
cpg	165.65	J/mol×K	557.12	Joback Method
cpg	171.21	J/mol×K	593.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C3448564&Units=SI

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

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