1-Propyne, 3-[(1-methylethyl)thio]-

Other names:	Sulfide, isopropyl 2-propynyl
	3-(Isopropylsulfanyl)-1-propyne
	5-Methyl-4-thia-1-hexyne
	Isopropyl propargyl sulfide
Inchi:	InChI=1S/C6H10S/c1-4-5-7-6(2)3/h1,6H,5H2,2-3H3
InchiKey:	LIIXPZMKZWEJRJ-UHFFFAOYSA-N
Formula:	C6H10S
SMILES:	C#CCSC(C)C
Mol. weight [g/mol]:	114.21
CAS:	14272-25-4

Physical Properties

Property code	Value	Unit	Source
gf	253.39	kJ/mol	Joback Method
hf	161.32	kJ/mol	Joback Method
hfus	14.88	kJ/mol	Joback Method
hvap	35.24	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.761		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	833.00		NIST Webbook
rinpol	833.00		NIST Webbook
tb	395.14	K	Joback Method
tc	603.38	K	Joback Method
tf	223.75	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.17	J/mol×K	395.14	Joback Method
cpg	191.24	J/mol×K	429.85	Joback Method
cpg	200.84	J/mol×K	464.55	Joback Method

cpg	209.98	J/mol×K	499.26	Joback Method
cpg	218.68	J/mol×K	533.96	Joback Method
cpg	226.93	J/mol×K	568.67	Joback Method
cpg	234.77	J/mol×K	603.38	Joback Method

Sources

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=C14272254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume