Propargyl ethyl sulphide

Other names:	3-(Ethylsulfanyl)-1-propyne
	4-Thia-1-hexyne
	Ethyl propargyl sulfide
Inchi:	InChI=1S/C5H8S/c1-3-5-6-4-2/h1H,4-5H2,2H3
InchiKey:	HGRTUSIZMXOMCD-UHFFFAOYSA-N
Formula:	C5H8S
SMILES:	C#CCSCC
Mol. weight [g/mol]:	100.19

Physical Properties

Property code	Value	Unit	Source
af	0.1750		Cheméo Relay (1.0)
gf	247.41	kJ/mol	Joback Method
hf	199.40	kJ/mol	Cheméo Relay (1.0)
hfus	15.81	kJ/mol	Joback Method
hvap	38.86	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-1.39		Cheméo Relay (1.0)
logp	1.373		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
rinpol	782.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	782.00		NIST Webbook
tb	403.88	K	Cheméo Relay (1.0)
tc	580.17	K	Cheméo Relay (1.0)
tf	174.37	K	Cheméo Relay (1.0)
vc	0.299	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.79	J/mol×K	372.70	Joback Method
cpg	154.92	J/mol×K	406.83	Joback Method

cpg	162.68	J/mol×K	440.95	Joback Method
cpg	170.09	J/mol×K	475.08	Joback Method
cpg	177.15	J/mol×K	509.21	Joback Method
cpg	183.88	J/mol×K	543.34	Joback Method
cpg	190.28	J/mol×K	577.46	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=C7310921&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.