

4-Ethylthio-3-buten-1-yne

Inchi:	InChI=1S/C6H8S/c1-3-5-6-7-4-2/h1,5-6H,4H2,2H3
InchiKey:	JQPJGIDORMRFQK-UHFFFAOYSA-N
Formula:	C6H8S
SMILES:	C#CC=CSCC
Mol. weight [g/mol]:	112.19
CAS:	1609-42-3

Physical Properties

Property code	Value	Unit	Source
gf	336.05	kJ/mol	Joback Method
hf	283.82	kJ/mol	Joback Method
hfus	18.60	kJ/mol	Joback Method
hvap	35.58	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.886		Crippen Method
mcvol	98.850	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	399.74	K	Joback Method
tc	613.97	K	Joback Method
tf	233.67	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.84	J/molxK	399.74	Joback Method
cpg	175.13	J/molxK	435.44	Joback Method
cpg	183.87	J/molxK	471.15	Joback Method
cpg	192.09	J/molxK	506.85	Joback Method
cpg	199.82	J/molxK	542.56	Joback Method
cpg	207.09	J/molxK	578.26	Joback Method
cpg	213.92	J/molxK	613.97	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=C1609423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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