2-propyne-1-thiol

Inchi: InChI=1S/C3H4S/c1-2-3-4/h1,4H,3H2
InchiKey: BHLUERUPCAAQGF-UHFFFAOYSA-N
Formula: C3H4S
SMILES: C#CCS
Mol. weight [g/mol]: 72.13

Physical Properties

Property code	Value	Unit	Source
gf	226.84	kJ/mol	Joback Method
hf	225.13	kJ/mol	Joback Method
hfus	10.54	kJ/mol	Joback Method
hvap	28.87	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.549		Crippen Method
mcvol	60.880	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
rinpol	611.00		NIST Webbook
rinpol	611.00		NIST Webbook
tb	321.02	K	Joback Method
tc	527.08	K	Joback Method
tf	207.00	K	Joback Method
vc	0.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.51	J/mol×K	321.02	Joback Method
cpg	90.05	J/mol×K	355.36	Joback Method
cpg	94.34	J/mol×K	389.71	Joback Method
cpg	98.39	J/mol×K	424.05	Joback Method
cpg	102.21	J/mol×K	458.39	Joback Method
cpg	105.82	J/mol×K	492.74	Joback Method
cpg	109.23	J/mol×K	527.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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