(allylthio)acetaldehyde

Other names: 2-[Allylthio]ethanal
Inchi: InChI=1S/C5H8OS/c1-2-4-7-5-3-6/h2-3H,1,4-5H2
InchiKey: UDPDMDAUIWISCF-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: C=CCSCC=O
Mol. weight [g/mol]: 116.18

Physical Properties

Property code	Value	Unit	Source
gf	12.66	kJ/mol	Joback Method
hf	-64.81	kJ/mol	Joback Method
hfus	13.84	kJ/mol	Joback Method
hvap	39.59	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.105		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	901.00		NIST Webbook
ripol	1495.00		NIST Webbook
tb	427.92	K	Joback Method
tc	629.86	K	Joback Method
tf	220.75	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.19	J/mol×K	427.92	Joback Method
cpg	179.60	J/mol×K	461.58	Joback Method
cpg	187.62	J/mol×K	495.23	Joback Method
cpg	195.25	J/mol×K	528.89	Joback Method
cpg	202.50	J/mol×K	562.55	Joback Method
cpg	209.38	J/mol×K	596.20	Joback Method
cpg	215.91	J/mol×K	629.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222627&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume