allyl thiopropanal

Other names: 3-(allylthio)propanal
Inchi: InChI=1S/C6H10OS/c1-2-5-8-6-3-4-7/h2,4H,1,3,5-6H2
InchiKey: AXZSEPBLUIEYQI-UHFFFAOYSA-N
Formula: C6H10OS
SMILES: C=CCSCCC=O
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
gf	21.08	kJ/mol	Joback Method
hf	-85.45	kJ/mol	Joback Method
hfus	16.43	kJ/mol	Joback Method
hvap	41.82	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.495		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1042.00		NIST Webbook
rinpol	1042.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1644.00		NIST Webbook
tb	450.80	K	Joback Method
tc	650.46	K	Joback Method
tf	232.02	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.90	J/mol×K	450.80	Joback Method
cpg	218.68	J/mol×K	484.08	Joback Method
cpg	228.00	J/mol×K	517.35	Joback Method
cpg	236.87	J/mol×K	550.63	Joback Method

cpg	245.30	J/mol×K	583.91	Joback Method
cpg	253.29	J/mol×K	617.19	Joback Method
cpg	260.87	J/mol×K	650.46	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=R222543&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume