allyl thioacetate

Inchi: InChI=1S/C5H8OS/c1-3-4-7-5(2)6/h3H,1,4H2,2H3
InchiKey: MIRAUQNBKACECA-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: C=CCSC(C)=O
Mol. weight [g/mol]: 116.18

Physical Properties

Property code	Value	Unit	Source
gf	-16.74	kJ/mol	Joback Method
hf	-91.81	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.62	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.452		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	835.00		NIST Webbook
rinpol	835.00		NIST Webbook
tb	433.13	K	Joback Method
tc	640.84	K	Joback Method
tf	228.68	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.03	J/mol×K	433.13	Joback Method
cpg	177.75	J/mol×K	467.75	Joback Method
cpg	186.05	J/mol×K	502.37	Joback Method
cpg	193.95	J/mol×K	536.98	Joback Method
cpg	201.46	J/mol×K	571.60	Joback Method
cpg	208.57	J/mol×K	606.22	Joback Method
cpg	215.30	J/mol×K	640.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R148346&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume