Propionic acid, 3-(allylthio)-

Other names:	3-(Allylsulfanyl)propanoic acid
	Propanoic acid, 3-(2-propenylthio)
Inchi:	InChI=1S/C6H10O2S/c1-2-4-9-5-3-6(7)8/h2H,1,3-5H2,(H,7,8)
InchiKey:	PPARCULXOKUJAV-UHFFFAOYSA-N
Formula:	C6H10O2S
SMILES:	C=CCSCCC(=O)O
Mol. weight [g/mol]:	146.21
CAS:	23349-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-145.14	kJ/mol	Joback Method
hf	-264.68	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.380		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	548.19	K	Joback Method
tc	741.05	K	Joback Method
tf	300.77	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.60	J/mol×K	548.19	Joback Method
cpg	258.20	J/mol×K	580.33	Joback Method
cpg	266.37	J/mol×K	612.48	Joback Method
cpg	274.12	J/mol×K	644.62	Joback Method
cpg	281.45	J/mol×K	676.77	Joback Method
cpg	288.39	J/mol×K	708.91	Joback Method
cpg	294.93	J/mol×K	741.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23349986&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume