3-Sulfanyl-2-ethylpropanal

Inchi: InChI=1S/C5H10OS/c1-2-5(3-6)4-7/h3,5,7H,2,4H2,1H3
InchiKey: FTNPNLVUSQKWBD-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CCC(C=O)CS
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-81.35	kJ/mol	Joback Method
hf	-198.91	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	39.79	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	1.141		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	931.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	424.88	K	Joback Method
tc	627.10	K	Joback Method
tf	209.57	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.44	J/mol×K	424.88	Joback Method
cpg	194.90	J/mol×K	458.58	Joback Method
cpg	203.92	J/mol×K	492.29	Joback Method
cpg	212.51	J/mol×K	525.99	Joback Method
cpg	220.67	J/mol×K	559.70	Joback Method
cpg	228.43	J/mol×K	593.40	Joback Method
cpg	235.78	J/mol×K	627.10	Joback Method

Sources

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=R621257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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