2-Sulfanylethyl acetate

Inchi: InChI=1S/C4H8O2S/c1-4(5)6-2-3-7/h7H,2-3H2,1H3
InchiKey: YDLAHBBJAGGIJZ-UHFFFAOYSA-N
Formula: C4H8O2S
SMILES: CC(=O)OCCS
Mol. weight [g/mol]: 120.17

Physical Properties

Property code	Value	Unit	Source
gf	-221.73	kJ/mol	Joback Method
hf	-332.21	kJ/mol	Joback Method
hfus	12.94	kJ/mol	Joback Method
hvap	40.39	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.479		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
rinpol	880.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	880.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1454.00		NIST Webbook
tb	430.07	K	Joback Method
tc	634.41	K	Joback Method
tf	243.46	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.85	J/mol×K	430.07	Joback Method
cpg	174.67	J/mol×K	464.13	Joback Method
cpg	182.21	J/mol×K	498.18	Joback Method
cpg	189.48	J/mol×K	532.24	Joback Method
cpg	196.47	J/mol×K	566.30	Joback Method

cpg	203.17	J/mol×K	600.36	Joback Method
cpg	209.57	J/mol×K	634.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613617&Units=SI

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