2-(Methylthiomethyl)ethanal

Inchi: InChI=1S/C4H8OS2/c1-6-4-7-3-2-5/h2H,3-4H2,1H3
InchiKey: BZVKQCXTDPCULV-UHFFFAOYSA-N
Formula: C4H8OS2
SMILES: CSCSCC=O
Mol. weight [g/mol]: 136.24

Physical Properties

Property code	Value	Unit	Source
gf	-50.48	kJ/mol	Joback Method
hf	-127.73	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.239		Crippen Method
mcvol	101.490	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
ripol	1915.00		NIST Webbook
ripol	1915.00		NIST Webbook
tb	477.14	K	Joback Method
tc	700.94	K	Joback Method
tf	245.64	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.97	J/mol×K	477.14	Joback Method
cpg	197.41	J/mol×K	514.44	Joback Method
cpg	205.46	J/mol×K	551.74	Joback Method
cpg	213.12	J/mol×K	589.04	Joback Method
cpg	220.38	J/mol×K	626.34	Joback Method
cpg	227.23	J/mol×K	663.64	Joback Method
cpg	233.67	J/mol×K	700.94	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=R504088&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume