2-thiapentanal

Inchi: InChI=1S/C4H8OS/c1-2-3-6-4-5/h4H,2-3H2,1H3
InchiKey: AIDJKHXHGBQDPE-UHFFFAOYSA-N
Formula: C4H8OS
SMILES: CCCSC=O
Mol. weight [g/mol]: 104.17

Physical Properties

Property code	Value	Unit	Source
gf	-83.60	kJ/mol	Joback Method
hf	-169.60	kJ/mol	Joback Method
hfus	12.53	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	1.320		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	870.00		NIST Webbook
tb	408.36	K	Joback Method
tc	607.86	K	Joback Method
tf	211.24	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.29	J/mol×K	408.36	Joback Method
cpg	158.00	J/mol×K	441.61	Joback Method
cpg	165.40	J/mol×K	474.86	Joback Method
cpg	172.50	J/mol×K	508.11	Joback Method
cpg	179.29	J/mol×K	541.36	Joback Method
cpg	185.79	J/mol×K	574.61	Joback Method
cpg	191.99	J/mol×K	607.86	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=R226416&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume