4-Mercaptopentan-2-one

Inchi: InChI=1S/C5H10OS/c1-4(6)3-5(2)7/h5,7H,3H2,1-2H3
InchiKey: KHIPEWLRUGVKIC-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CC(=O)CC(C)S
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-110.75	kJ/mol	Joback Method
hf	-225.91	kJ/mol	Joback Method
hfus	10.82	kJ/mol	Joback Method
hvap	39.82	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.284		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	884.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	884.00		NIST Webbook
tb	430.09	K	Joback Method
tc	638.12	K	Joback Method
tf	217.50	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.43	J/mol×K	430.09	Joback Method
cpg	193.22	J/mol×K	464.76	Joback Method
cpg	202.55	J/mol×K	499.43	Joback Method
cpg	211.43	J/mol×K	534.10	Joback Method
cpg	219.86	J/mol×K	568.78	Joback Method
cpg	227.86	J/mol×K	603.45	Joback Method
cpg	235.44	J/mol×K	638.12	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=R603155&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume