4-Methylthio-2-butanone

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

Physical Properties

Property code	Value	Unit	Source
gf	-104.58	kJ/mol	Joback Method
hf	-217.24	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.329		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
ripol	1532.00		NIST Webbook
tb	436.45	K	Joback Method
tc	639.57	K	Joback Method
tf	230.44	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.53	J/mol×K	436.45	Joback Method
cpg	194.04	J/mol×K	470.30	Joback Method
cpg	203.15	J/mol×K	504.16	Joback Method
cpg	211.86	J/mol×K	538.01	Joback Method
cpg	220.19	J/mol×K	571.86	Joback Method
cpg	228.12	J/mol×K	605.72	Joback Method
cpg	235.68	J/mol×K	639.57	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=R640976&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume