

Methylthio-2-propanone

Other names:	(Methylthio)acetone 1-Methylthio-2-propanone 2-Propanone, 1-(methylthio)- 1-methylsulfanylpropan-2-one
Inchi:	InChI=1S/C4H8OS/c1-4(5)3-6-2/h3H2,1-2H3
InchiKey:	UKFADLGENFFWHR-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	CSCC(C)=O
Mol. weight [g/mol]:	104.17
CAS:	14109-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-113.00	kJ/mol	Joback Method
hf	-196.60	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	38.06	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.938		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
tb	413.57	K	Joback Method
tc	618.94	K	Joback Method
tf	219.17	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.97	J/mol×K	413.57	Joback Method
cpg	155.97	J/mol×K	447.80	Joback Method

cpg	163.66	J/mol×K	482.03	Joback Method
cpg	171.03	J/mol×K	516.25	Joback Method
cpg	178.09	J/mol×K	550.48	Joback Method
cpg	184.83	J/mol×K	584.71	Joback Method
cpg	191.25	J/mol×K	618.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14109729&Units=SI
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

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

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