

1-(Methylthio)-3-pentanone

Other names:	3-Pentanone, 1-(methylthio)- 1-(Methylthio)pentan-3-one
Inchi:	InChI=1S/C6H12OS/c1-3-6(7)4-5-8-2/h3-5H2,1-2H3
InchiKey:	LEZZIANNWFYCND-UHFFFAOYSA-N
Formula:	C6H12OS
SMILES:	CCC(=O)CCSC
Mol. weight [g/mol]:	132.22
CAS:	66735-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.16	kJ/mol	Joback Method
hf	-237.88	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.719		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1052.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	459.33	K	Joback Method
tc	660.04	K	Joback Method
tf	241.71	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.40	J/mol×K	459.33	Joback Method
cpg	234.25	J/mol×K	492.78	Joback Method
cpg	244.63	J/mol×K	526.23	Joback Method
cpg	254.54	J/mol×K	559.69	Joback Method
cpg	264.00	J/mol×K	593.14	Joback Method
cpg	273.01	J/mol×K	626.59	Joback Method
cpg	281.57	J/mol×K	660.04	Joback Method

Sources

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=C66735691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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