

# Thioacetone

<b>Inchi:</b>	InChI=1S/C3H6S/c1-3(2)4/h1-2H3
<b>InchiKey:</b>	JTNXQVCPQMQLHK-UHFFFAOYSA-N
<b>Formula:</b>	C3H6S
<b>SMILES:</b>	CC(C)=S
<b>Mol. weight [g/mol]:</b>	74.14
<b>CAS:</b>	4756-05-2

## Physical Properties

Property code	Value	Unit	Source
gf	91.44	kJ/mol	Joback Method
hf	41.25	kJ/mol	Joback Method
hfus	8.13	kJ/mol	Joback Method
hvap	29.00	kJ/mol	Joback Method
ie	8.60 ± 0.05	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-1.43		Crippen Method
logp	1.396		Crippen Method
mcvol	65.180	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	338.08	K	Joback Method
tc	535.53	K	Joback Method
tf	157.84	K	Joback Method
vc	0.239	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.49	J/molxK	338.08	Joback Method
cpg	97.97	J/molxK	370.99	Joback Method
cpg	104.01	J/molxK	403.90	Joback Method
cpg	109.63	J/molxK	436.80	Joback Method
cpg	114.86	J/molxK	469.71	Joback Method
cpg	119.74	J/molxK	502.62	Joback Method
cpg	124.28	J/molxK	535.53	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4756052&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4756052&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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