

# 3-Penten-2-one, 1,1,1-trifluoro-4-mercapto

<b>Inchi:</b>	InChI=1S/C5H5F3OS/c1-3(10)2-4(9)5(6,7)8/h2,10H,1H3/b3-2-
<b>InchiKey:</b>	RCKPNIPOQOBBDS-IHWYPQMZSA-N
<b>Formula:</b>	C5H5F3OS
<b>SMILES:</b>	CC(S)=CC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	170.15
<b>CAS:</b>	7141-17-5

## Physical Properties

Property code	Value	Unit	Source
gf	-618.23	kJ/mol	Joback Method
hf	-710.28	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	36.50	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.951		Crippen Method
mcvol	100.240	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	429.15	K	Joback Method
tc	626.26	K	Joback Method
tf	217.65	K	Joback Method
vc	0.400	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.92	J/molxK	429.15	Joback Method
cpg	203.79	J/molxK	462.00	Joback Method
cpg	212.00	J/molxK	494.85	Joback Method
cpg	219.58	J/molxK	527.71	Joback Method
cpg	226.59	J/molxK	560.56	Joback Method
cpg	233.05	J/molxK	593.41	Joback Method
cpg	239.01	J/molxK	626.26	Joback Method

# Sources

<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=C7141175&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7141175&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

# 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>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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