

# (2-Tetrahydropyranylmercapto)-acethydroxamic acid

InChI:	InChI=1S/C7H13NO3S/c9-6(8-10)5-12-7-3-1-2-4-11-7/h7,10H,1-5H2,(H,8,9)
InChIKey:	AOXNRFNBOXSPNC-UHFFFAOYSA-N
Formula:	C7H13NO3S
SMILES:	O=C(CSC1CCCCO1)NO
Mol. weight [g/mol]:	191.25
CAS:	772-68-9

## Physical Properties

Property code	Value	Unit	Source
gf	-196.84	kJ/mol	Joback Method
hf	-434.96	kJ/mol	Joback Method
hfus	28.62	kJ/mol	Joback Method
hvap	72.79	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.752		Crippen Method
mvol	138.270	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	671.06	K	Joback Method
tc	888.52	K	Joback Method
tf	400.41	K	Joback Method
vc	0.495	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.50	J/molxK	671.06	Joback Method
cpg	388.56	J/molxK	707.30	Joback Method
cpg	399.78	J/molxK	743.55	Joback Method
cpg	410.16	J/molxK	779.79	Joback Method
cpg	419.73	J/molxK	816.04	Joback Method
cpg	428.49	J/molxK	852.28	Joback Method
cpg	436.46	J/molxK	888.52	Joback Method

# Sources

<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=C772689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C772689&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>

# 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>hvac:</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>mccvol:</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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