

# Pentanethioic acid, S-ethyl ester

<b>Other names:</b>	Valeric acid, thio-, S-ethyl ester S-ethyl pentanethioate
<b>Inchi:</b>	InChI=1S/C7H14OS/c1-3-5-6-7(8)9-4-2/h3-6H2,1-2H3
<b>InchiKey:</b>	CGRFTVFWSJEHCI-UHFFFAOYSA-N
<b>Formula:</b>	C7H14OS
<b>SMILES:</b>	CCCCC(=O)SCC
<b>Mol. weight [g/mol]:</b>	146.25
<b>CAS:</b>	2432-92-0

## Physical Properties

Property code	Value	Unit	Source
gf	-87.74	kJ/mol	Joback Method
hf	-258.52	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.456		Crippen Method
mvol	127.410	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	938.00		NIST Webbook
tb	482.21	K	Joback Method
tc	680.42	K	Joback Method
tf	252.98	K	Joback Method
vc	0.487	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.46	J/molxK	482.21	Joback Method
cpg	276.49	J/molxK	515.24	Joback Method
cpg	288.00	J/molxK	548.28	Joback Method
cpg	298.98	J/molxK	581.31	Joback Method
cpg	309.45	J/molxK	614.35	Joback Method
cpg	319.41	J/molxK	647.38	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=C2432920&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432920&amp;Units=SI</a>
<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>

## 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>rinpol:</b>	Non-polar retention indices
<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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