

# Octanoic acid, 6,8-dimercapto-

<b>Other names:</b>	Dihydrolipoic acid
<b>Inchi:</b>	InChI=1S/C8H16O2S2/c9-8(10)4-2-1-3-7(12)5-6-11/h7,11-12H,1-6H2,(H,9,10)
<b>InchiKey:</b>	IZFHEQBZOYJLPK-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2S2
<b>SMILES:</b>	O=C(O)CCCCC(S)CCS
<b>Mol. weight [g/mol]:</b>	208.34
<b>CAS:</b>	462-20-4

## Physical Properties

Property code	Value	Unit	Source
gf	-192.92	kJ/mol	Joback Method
hf	-401.58	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hvap	69.91	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.250		Crippen Method
mcvol	163.720	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	653.77	K	Joback Method
tc	858.12	K	Joback Method
tf	348.59	K	Joback Method
vc	0.611	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.51	J/mol×K	653.77	Joback Method
cpg	415.65	J/mol×K	687.83	Joback Method
cpg	426.16	J/mol×K	721.89	Joback Method
cpg	436.05	J/mol×K	755.95	Joback Method
cpg	445.36	J/mol×K	790.00	Joback Method
cpg	454.09	J/mol×K	824.06	Joback Method
cpg	462.28	J/mol×K	858.12	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C462204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C462204&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>
<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>

# 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>hvp:</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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