

# n-Dodecyl thioglycolate

<b>Other names:</b>	Acetic acid, mercapto-, dodecyl ester dodecyl mercaptoacetate
<b>Inchi:</b>	InChI=1S/C14H28O2S/c1-2-3-4-5-6-7-8-9-10-11-12-16-14(15)13-17/h17H,2-13H2,1H3
<b>InchiKey:</b>	TVMDUMQNXXNGMG-UHFFFAOYSA-N
<b>Formula:</b>	C14H28O2S
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CS
<b>Mol. weight [g/mol]:</b>	260.44
<b>CAS:</b>	3746-39-2

## Physical Properties

Property code	Value	Unit	Source
gf	-137.53	kJ/mol	Joback Method
hf	-538.61	kJ/mol	Joback Method
hfus	38.84	kJ/mol	Joback Method
hvap	62.65	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.380		Crippen Method
mvol	231.910	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
tb	658.87	K	Joback Method
tc	841.40	K	Joback Method
tf	356.16	K	Joback Method
vc	0.897	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.71	J/molxK	658.87	Joback Method
cpg	645.51	J/molxK	689.29	Joback Method
cpg	661.52	J/molxK	719.71	Joback Method
cpg	676.75	J/molxK	750.14	Joback Method
cpg	691.22	J/molxK	780.56	Joback Method
cpg	704.94	J/molxK	810.98	Joback Method
cpg	717.93	J/molxK	841.40	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3746392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3746392&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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