

# Ethiolate

<b>Other names:</b>	Carbamothioic acid, diethyl-, S-ethyl ester Carbamic acid, diethylthio-, S-ethyl ester S-Ethyl N,N-diethylthiocarbamate S-Ethyl diethylcarbamothioate S-Ethyl diethylthiocarbamate S-15076 Etirox
<b>Inchi:</b>	InChI=1S/C7H15NOS/c1-4-8(5-2)7(9)10-6-3/h4-6H2,1-3H3
<b>InchiKey:</b>	WARIWGPBHKPYON-UHFFFAOYSA-N
<b>Formula:</b>	C7H15NOS
<b>SMILES:</b>	CCSC(=O)N(CC)CC
<b>Mol. weight [g/mol]:</b>	161.26
<b>CAS:</b>	2941-55-1

## Physical Properties

Property code	Value	Unit	Source
gf	23.04	kJ/mol	Joback Method
hf	-190.99	kJ/mol	Joback Method
hfus	22.64	kJ/mol	Joback Method
hvap	46.78	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.201		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	494.65	K	Joback Method
tc	690.36	K	Joback Method
tf	285.45	K	Joback Method
vc	0.505	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.64	J/mol×K	494.65	Joback Method
cpg	309.57	J/mol×K	527.27	Joback Method

cpg	321.88	J/mol×K	559.89	Joback Method
cpg	333.57	J/mol×K	592.51	Joback Method
cpg	344.66	J/mol×K	625.13	Joback Method
cpg	355.17	J/mol×K	657.74	Joback Method
cpg	365.11	J/mol×K	690.36	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=C2941551&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2941551&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>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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