

# Ethanesulfinic acid, methyl ester

<b>Other names:</b>	Methyl ethanesulfinate
<b>Inchi:</b>	InChI=1S/C3H8O2S/c1-3-6(4)5-2/h3H2,1-2H3
<b>InchiKey:</b>	UTOWKUXZEJXEMP-UHFFFAOYSA-N
<b>Formula:</b>	C3H8O2S
<b>SMILES:</b>	CCS(=O)OC
<b>Mol. weight [g/mol]:</b>	108.16
<b>CAS:</b>	31401-21-5

## Physical Properties

Property code	Value	Unit	Source
gf	-348.33	kJ/mol	Joback Method
hf	-443.21	kJ/mol	Joback Method
hfus	12.47	kJ/mol	Joback Method
hvap	37.41	kJ/mol	Joback Method
log10ws	0.21		Crippen Method
logp	0.316		Crippen Method
mcvol	81.220	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
rinpol	798.00		NIST Webbook
tb	348.74	K	Joback Method
tc	526.14	K	Joback Method
tf	182.28	K	Joback Method
vc	0.311	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.42	J/molxK	348.74	Joback Method
cpg	142.14	J/molxK	378.31	Joback Method
cpg	148.76	J/molxK	407.87	Joback Method
cpg	155.26	J/molxK	437.44	Joback Method
cpg	161.62	J/molxK	467.01	Joback Method
cpg	167.85	J/molxK	496.57	Joback Method
cpg	173.92	J/molxK	526.14	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C31401215&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31401215&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>rinp:</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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