

# Acetic acid, sulfo-, diethyl ester

Inchi:	InChI=1S/C6H12O5S/c1-3-10-6(7)5-12(8,9)11-4-2/h3-5H2,1-2H3
InchiKey:	VWKJYZVWQUJSEH-UHFFFAOYSA-N
Formula:	C6H12O5S
SMILES:	CCOC(=O)CS(=O)(=O)OCC
Mol. weight [g/mol]:	196.22
CAS:	59376-54-4

## Physical Properties

Property code	Value	Unit	Source
gf	-807.82	kJ/mol	Joback Method
hf	-997.54	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	59.15	kJ/mol	Joback Method
log10ws	-0.11		Crippen Method
logp	-0.084		Crippen Method
mcvol	136.800	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	483.17	K	Joback Method
tc	657.11	K	Joback Method
tf	290.33	K	Joback Method
vc	0.539	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.07	J/molxK	483.17	Joback Method
cpg	305.69	J/molxK	512.16	Joback Method
cpg	316.00	J/molxK	541.15	Joback Method
cpg	325.98	J/molxK	570.14	Joback Method
cpg	335.62	J/molxK	599.13	Joback Method
cpg	344.91	J/molxK	628.12	Joback Method
cpg	353.81	J/molxK	657.11	Joback Method

# Sources

<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=C59376544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C59376544&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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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