

# Menthol, methanesulfinate

<b>Inchi:</b>	InChI=1S/C11H22O2S/c1-8(2)10-6-5-9(3)7-11(10)13-14(4)12/h8-11H,5-7H2,1-4H3
<b>InchiKey:</b>	BLHQYXSQYFQSGP-UHFFFAOYSA-N
<b>Formula:</b>	C11H22O2S
<b>SMILES:</b>	CC1CCC(C(C)C)C(OS(C)=O)C1
<b>Mol. weight [g/mol]:</b>	218.36
<b>CAS:</b>	94487-99-7

## Physical Properties

Property code	Value	Unit	Source
gf	-274.38	kJ/mol	Joback Method
hf	-599.97	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	54.64	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.757		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
tb	541.55	K	Joback Method
tc	745.17	K	Joback Method
tf	256.34	K	Joback Method
vc	0.684	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.32	J/molxK	541.55	Joback Method
cpg	475.35	J/molxK	575.49	Joback Method
cpg	495.38	J/molxK	609.42	Joback Method
cpg	514.41	J/molxK	643.36	Joback Method
cpg	532.43	J/molxK	677.30	Joback Method
cpg	549.44	J/molxK	711.23	Joback Method
cpg	565.43	J/molxK	745.17	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=C94487997&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94487997&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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