

# Benzenesulfinic-acid-

<b>Other names:</b>	benzenesulphinic acid
<b>Inchi:</b>	InChI=1S/C6H6O2S/c7-9(8)6-4-2-1-3-5-6/h1-5H,(H,7,8)
<b>InchiKey:</b>	JEHKKBHWRAXMCH-UHFFFAOYSA-N
<b>Formula:</b>	C6H6O2S
<b>SMILES:</b>	O=S(O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	142.18
<b>CAS:</b>	618-41-7

## Physical Properties

Property code	Value	Unit	Source
gf	-242.48	kJ/mol	Joback Method
hf	-288.61	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	1.267		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
pc	6056.11	kPa	Joback Method
tb	513.82	K	Joback Method
tc	723.75	K	Joback Method
tf	281.10	K	Joback Method
vc	0.372	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.80	J/mol×K	513.82	Joback Method
cpg	207.70	J/mol×K	548.81	Joback Method
cpg	216.05	J/mol×K	583.80	Joback Method
cpg	223.85	J/mol×K	618.78	Joback Method
cpg	231.11	J/mol×K	653.77	Joback Method
cpg	237.85	J/mol×K	688.76	Joback Method
cpg	244.09	J/mol×K	723.75	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C618417&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C618417&amp;Units=SI</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>h vap:</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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