

# 3-Chlorosalicylic acid

<b>Other names:</b>	Benzoic acid, 3-chloro-2-hydroxy- Salicylic acid, 3-chloro-
<b>Inchi:</b>	InChI=1S/C7H5ClO3/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3,9H,(H,10,11)
<b>InchiKey:</b>	PPINMMULCRBDOS-UHFFFAOYSA-N
<b>Formula:</b>	C7H5ClO3
<b>SMILES:</b>	O=C(O)c1cccc(Cl)c1O
<b>Mol. weight [g/mol]:</b>	172.57
<b>CAS:</b>	1829-32-9

## Physical Properties

Property code	Value	Unit	Source
gf	-321.45	kJ/mol	Joback Method
hf	-420.61	kJ/mol	Joback Method
hfus	23.21	kJ/mol	Joback Method
hvap	74.94	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.744		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	655.32	K	Joback Method
tc	879.90	K	Joback Method
tf	459.98	K	Joback Method
vc	0.359	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.69	J/molxK	655.32	Joback Method
cpg	256.05	J/molxK	692.75	Joback Method
cpg	261.95	J/molxK	730.18	Joback Method
cpg	267.47	J/molxK	767.61	Joback Method
cpg	272.67	J/molxK	805.04	Joback Method

cpg	277.63	J/molxK	842.47	Joback Method
cpg	282.40	J/molxK	879.90	Joback Method
dvisc	0.0004187	Paxs	459.98	Joback Method
dvisc	0.0001872	Paxs	492.54	Joback Method
dvisc	0.0000925	Paxs	525.09	Joback Method
dvisc	0.0000496	Paxs	557.65	Joback Method
dvisc	0.0000285	Paxs	590.21	Joback Method
dvisc	0.0000174	Paxs	622.76	Joback Method
dvisc	0.0000111	Paxs	655.32	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=C1829329&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1829329&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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