

# C8H7ClO2

<b>Inchi:</b>	InChI=1S/C8H7ClO2/c9-5-6-2-1-3-7(4-6)8(10)11/h1-4H,5H2,(H,10,11)
<b>InchiKey:</b>	PBSUMBYSVFTMNG-UHFFFAOYSA-N
<b>Formula:</b>	C8H7ClO2
<b>SMILES:</b>	O=C(O)c1cccc(CCl)c1
<b>Mol. weight [g/mol]:</b>	170.59
<b>CAS:</b>	31719-77-4

## Physical Properties

Property code	Value	Unit	Source
gf	-158.41	kJ/mol	Joback Method
hf	-263.94	kJ/mol	Joback Method
hfus	20.01	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.124		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	597.58	K	Joback Method
tc	809.04	K	Joback Method
tf	359.53	K	Joback Method
vc	0.450	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.49	J/molxK	597.58	Joback Method
cpg	266.08	J/molxK	632.82	Joback Method
cpg	274.10	J/molxK	668.07	Joback Method
cpg	281.58	J/molxK	703.31	Joback Method
cpg	288.55	J/molxK	738.55	Joback Method
cpg	295.02	J/molxK	773.80	Joback Method
cpg	301.02	J/molxK	809.04	Joback Method
dvisc	0.0036481	Paxs	359.53	Joback Method
dvisc	0.0015134	Paxs	399.21	Joback Method

dvisc	0.0007361	Paxs	438.88	Joback Method
dvisc	0.0004034	Paxs	478.55	Joback Method
dvisc	0.0002425	Paxs	518.23	Joback Method
dvisc	0.0001567	Paxs	557.90	Joback Method
dvisc	0.0001073	Paxs	597.58	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=C31719774&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31719774&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>mccvol:</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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