

# 2-Propanol, 1-chloro-3-propoxy-

Inchi:	InChI=1S/C6H13ClO2/c1-2-3-9-5-6(8)4-7/h6,8H,2-5H2,1H3
InchiKey:	BJKFQZKSICPHSR-UHFFFAOYSA-N
Formula:	C6H13ClO2
SMILES:	CCCOCC(O)CCl
Mol. weight [g/mol]:	152.62
CAS:	6943-58-4

## Physical Properties

Property code	Value	Unit	Source
gf	-256.55	kJ/mol	Joback Method
hf	-472.64	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	52.04	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	1.013		Crippen Method
mvol	119.380	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	488.27	K	Joback Method
tc	658.77	K	Joback Method
tf	255.35	K	Joback Method
vc	0.452	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.76	J/mol×K	488.27	Joback Method
cpg	265.10	J/mol×K	516.69	Joback Method
cpg	274.09	J/mol×K	545.10	Joback Method
cpg	282.76	J/mol×K	573.52	Joback Method
cpg	291.09	J/mol×K	601.94	Joback Method
cpg	299.09	J/mol×K	630.36	Joback Method
cpg	306.77	J/mol×K	658.77	Joback Method
dvisc	0.0369054	Paxs	255.35	Joback Method
dvisc	0.0081343	Paxs	294.17	Joback Method

dvisc	0.0025508	Paxs	332.99	Joback Method
dvisc	0.0010191	Paxs	371.81	Joback Method
dvisc	0.0004843	Paxs	410.63	Joback Method
dvisc	0.0002617	Paxs	449.45	Joback Method
dvisc	0.0001559	Paxs	488.27	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=C6943584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6943584&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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