3-Chloro-1-propanol

Other names: 1-Chloro-3-hydroxypropane
1-Chloro-3-propanol
3-Chloro-1-hydroxypropane
3-Chloropropane-1-ol
3-Chloropropanol
3-Chloropropanol-1
3-Chlorpropan-1-ol
3-chloropropan-1-ol
NSC 60190
Propanol, 3-chloro-
Trimethylene chlorohydrin
UN 2849

Inchi: InChI=1S/C3H7ClO/c4-2-1-3-5/h5H,1-3H2

InchiKey: LAMUXTNQCICZQX-UHFFFAOYSA-N

Formula: C3H7ClO

SMILES: OCCCCl

Mol. weight [g/mol]: 94.54

Physical Properties

Property code	Value	Unit	Source
af	0.5887		Cheméo Relay (1.0)
hf	-300.75	kJ/mol	Cheméo Relay (1.0)
hfus	11.81	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Cheméo Relay (1.0)
ie	10.70	eV	NIST Webbook
ie	10.35	eV	NIST Webbook
log10ws	0.35		Cheméo Relay (1.0)
logp	0.608		Crippen Method
mcvol	71.240	ml/mol	McGowan Method
pc	4749.69	kPa	Joback Method
tb	434.20	K	NIST Webbook
tb	434.00 ± 1.00	K	NIST Webbook
tc	654.77	K	Cheméo Relay (1.0)
tf	193.36	K	Cheméo Relay (1.0)
vc	0.249	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.06	J/mol×K	397.65	Joback Method
cpg	127.58	J/mol×K	426.00	Joback Method
cpg	132.89	J/mol×K	454.35	Joback Method
cpg	137.99	J/mol×K	482.70	Joback Method
cpg	142.89	J/mol×K	511.05	Joback Method
cpg	147.59	J/mol×K	539.41	Joback Method
cpg	152.09	J/mol×K	567.76	Joback Method
dvisc	0.0795736	Pa×s	214.31	Joback Method
dvisc	0.0187350	Pa×s	244.87	Joback Method
dvisc	0.0060801	Pa×s	275.42	Joback Method
dvisc	0.0024705	Pa×s	305.98	Joback Method
dvisc	0.0011822	Pa×s	336.54	Joback Method
dvisc	0.0006395	Pa×s	367.09	Joback Method
dvisc	0.0003802	Pa×s	397.65	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.20	K	0.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Interaction of some hydrophobic amino acids, peptides, and protein with aqueous 3-chloro-1,2-propanediol and 3-chloro-1-propanol: Biophysical studies.: https://www.doi.org/10.1016/j.jct.2010.11.015

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627305&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume