

4-Chloro-1-butanol

Other names:	1-Butanol, 4-chloro- Tetramethylene chlorohydrin 4-Chloro-1-butane-ol 4-Chlorobutanol 4-Chlorbutan-1-ol 4-chlorobutan-1-ol
Inchi:	InChI=1S/C4H9ClO/c5-3-1-2-4-6/h6H,1-4H2
InchiKey:	HXHGULXINZUGJX-UHFFFAOYSA-N
Formula:	C4H9ClO
SMILES:	OCCCCCl
Mol. weight [g/mol]:	108.57
CAS:	928-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-165.95	kJ/mol	Joback Method
hf	-293.86	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	45.56	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	0.998		Crippen Method
mcvol	85.330	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	420.53	K	Joback Method
tc	589.86	K	Joback Method
tf	225.58	K	Joback Method
vc	0.328	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.84	J/mol×K	420.53	Joback Method
cpg	163.71	J/mol×K	448.75	Joback Method
cpg	170.30	J/mol×K	476.97	Joback Method

cpg	176.63	J/mol×K	505.20	Joback Method
cpg	182.70	J/mol×K	533.42	Joback Method
cpg	188.53	J/mol×K	561.64	Joback Method
cpg	194.11	J/mol×K	589.86	Joback Method
dvisc	0.0637141	Paxs	225.58	Joback Method
dvisc	0.0151132	Paxs	258.07	Joback Method
dvisc	0.0049457	Paxs	290.56	Joback Method
dvisc	0.0020262	Paxs	323.05	Joback Method
dvisc	0.0009772	Paxs	355.55	Joback Method
dvisc	0.0005325	Paxs	388.04	Joback Method
dvisc	0.0003187	Paxs	420.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.70	K	2.10	NIST Webbook
tbrp	360.50 ± 1.50	K	2.70	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C928518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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

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