

2-Butanol, 1-chloro-

Other names:	«alpha»-Butylene chlorohydrin 1-Chloro-2-butanol
Inchi:	InChI=1S/C4H9ClO/c1-2-4(6)3-5/h4,6H,2-3H2,1H3
InchiKey:	VNBFUGOVQMFIRN-UHFFFAOYSA-N
Formula:	C4H9ClO
SMILES:	CCC(O)CCl
Mol. weight [g/mol]:	108.57
CAS:	1873-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-168.39	kJ/mol	Joback Method
hf	-299.14	kJ/mol	Joback Method
hfus	10.88	kJ/mol	Joback Method
h vap	45.17	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	0.996		Crippen Method
m cvol	85.330	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	420.09	K	Joback Method
tc	593.20	K	Joback Method
tf	210.58	K	Joback Method
vc	0.322	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.93	J/mol×K	420.09	Joback Method
cpg	189.63	J/mol×K	564.35	Joback Method
cpg	183.64	J/mol×K	535.50	Joback Method
cpg	177.38	J/mol×K	506.65	Joback Method
cpg	170.85	J/mol×K	477.79	Joback Method
cpg	164.04	J/mol×K	448.94	Joback Method
cpg	195.36	J/mol×K	593.20	Joback Method

dvisc	0.0003069	Paxs	420.09	Joback Method
dvisc	0.0005398	Paxs	385.17	Joback Method
dvisc	0.0010623	Paxs	350.25	Joback Method
dvisc	0.0024290	Paxs	315.33	Joback Method
dvisc	0.0068239	Paxs	280.42	Joback Method
dvisc	0.0257191	Paxs	245.50	Joback Method
dvisc	0.1505149	Paxs	210.58	Joback Method

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=C1873252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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