

2-Propanol, 1-chloro-3-(2-butoxy)

Inchi:	InChI=1S/C7H15ClO2/c1-3-6(2)10-5-7(9)4-8/h6-7,9H,3-5H2,1-2H3
InchiKey:	ZHFMICGTLXOGMZ-UHFFFAOYSA-N
Formula:	C7H15ClO2
SMILES:	CCC(C)OCC(O)CCl
Mol. weight [g/mol]:	166.65

Physical Properties

Property code	Value	Unit	Source
gf	-250.57	kJ/mol	Joback Method
hf	-498.56	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.401		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinsol	1110.00		NIST Webbook
tb	510.71	K	Joback Method
tc	683.29	K	Joback Method
tf	251.62	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.61	J/molxK	510.71	Joback Method
cpg	309.22	J/molxK	539.47	Joback Method
cpg	319.42	J/molxK	568.24	Joback Method
cpg	329.22	J/molxK	597.00	Joback Method
cpg	338.62	J/molxK	625.76	Joback Method
cpg	347.63	J/molxK	654.53	Joback Method
cpg	356.25	J/molxK	683.29	Joback Method
dvisc	0.0578400	Paxs	251.62	Joback Method
dvisc	0.0097512	Paxs	294.80	Joback Method

dvisc	0.0025909	Paxs	337.98	Joback Method
dvisc	0.0009295	Paxs	381.16	Joback Method
dvisc	0.0004109	Paxs	424.35	Joback Method
dvisc	0.0002112	Paxs	467.53	Joback Method
dvisc	0.0001215	Paxs	510.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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