

2-Propanol, 1-chloro-3-methoxy-

Other names:	1-Chloro-3-methoxypropan-2-ol
Inchi:	InChI=1S/C4H9ClO2/c1-7-3-4(6)2-5/h4,6H,2-3H2,1H3
InchiKey:	FOLYKNXDLNPWGC-UHFFFAOYSA-N
Formula:	C4H9ClO2
SMILES:	COCC(O)CCl
Mol. weight [g/mol]:	124.57
CAS:	4151-97-7

Physical Properties

Property code	Value	Unit	Source
gf	-273.39	kJ/mol	Joback Method
hf	-431.36	kJ/mol	Joback Method
hfus	12.07	kJ/mol	Joback Method
hvap	47.58	kJ/mol	Joback Method
log10ws	-0.11		Crippen Method
logp	0.232		Crippen Method
mccvol	91.200	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	442.51	K	Joback Method
tc	615.48	K	Joback Method
tf	232.81	K	Joback Method
vc	0.340	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.00	J/molxK	442.51	Joback Method
cpg	183.98	J/molxK	471.34	Joback Method
cpg	190.74	J/molxK	500.17	Joback Method
cpg	197.27	J/molxK	529.00	Joback Method
cpg	203.57	J/molxK	557.83	Joback Method
cpg	209.64	J/molxK	586.66	Joback Method
cpg	215.49	J/molxK	615.48	Joback Method
dvisc	0.0605720	Paxs	232.81	Joback Method

dvisc	0.0130502	Paxs	267.76	Joback Method
dvisc	0.0040077	Paxs	302.71	Joback Method
dvisc	0.0015715	Paxs	337.66	Joback Method
dvisc	0.0007345	Paxs	372.61	Joback Method
dvisc	0.0003912	Paxs	407.56	Joback Method
dvisc	0.0002301	Paxs	442.51	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=C4151977&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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