

Propane, 3-chloro-1,1-dimethoxy-

Inchi:	InChI=1S/C5H11ClO2/c1-7-5(8-2)3-4-6/h5H,3-4H2,1-2H3
InchiKey:	DXWRNRRBDAQWDB-UHFFFAOYSA-N
Formula:	C5H11ClO2
SMILES:	COC(CCCI)OC
Mol. weight [g/mol]:	138.59
CAS:	35502-06-8

Physical Properties

Property code	Value	Unit	Source
gf	-233.15	kJ/mol	Joback Method
hf	-431.99	kJ/mol	Joback Method
hfus	11.76	kJ/mol	Joback Method
hvap	35.54	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	1.234		Crippen Method
mcvol	105.290	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	395.63	K	Joback Method
tc	573.32	K	Joback Method
tf	205.49	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.95	J/molxK	395.63	Joback Method
cpg	202.76	J/molxK	425.24	Joback Method
cpg	211.37	J/molxK	454.86	Joback Method
cpg	219.76	J/molxK	484.47	Joback Method
cpg	227.93	J/molxK	514.09	Joback Method
cpg	235.87	J/molxK	543.70	Joback Method
cpg	243.57	J/molxK	573.32	Joback Method
dvisc	0.0040967	Paxs	205.49	Joback Method
dvisc	0.0018358	Paxs	237.18	Joback Method

dvisc	0.0009940	Paxs	268.87	Joback Method
dvisc	0.0006125	Paxs	300.56	Joback Method
dvisc	0.0004140	Paxs	332.25	Joback Method
dvisc	0.0002995	Paxs	363.94	Joback Method
dvisc	0.0002283	Paxs	395.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	13.30	NIST Webbook
tbrp	324.20	K	2.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35502068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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