

Propane, 1-chloro-3-methoxy-

Other names:	1-chloro-3-methoxypropane
Inchi:	InChI=1S/C4H9ClO/c1-6-4-2-3-5/h2-4H2,1H3
InchiKey:	BQLHMMQUVJCTAN-UHFFFAOYSA-N
Formula:	C4H9ClO
SMILES:	COCCCCI
Mol. weight [g/mol]:	108.57
CAS:	36215-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-134.13	kJ/mol	Joback Method
hf	-273.85	kJ/mol	Joback Method
hfus	11.50	kJ/mol	Joback Method
hvap	31.29	kJ/mol	Joback Method
log10ws	-0.74		Crippen Method
logp	1.262		Crippen Method
mcvol	85.330	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	730.70		NIST Webbook
rinpol	726.20		NIST Webbook
tb	350.77	K	Joback Method
tc	524.29	K	Joback Method
tf	186.99	K	Joback Method
vc	0.327	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.39	J/molxK	350.77	Joback Method
cpg	146.57	J/molxK	379.69	Joback Method
cpg	153.56	J/molxK	408.61	Joback Method
cpg	160.36	J/molxK	437.53	Joback Method
cpg	166.96	J/molxK	466.45	Joback Method
cpg	173.37	J/molxK	495.37	Joback Method

cpg	179.58	J/molxK	524.29	Joback Method
dvisc	0.0030669	Paxs	186.99	Joback Method
dvisc	0.0015726	Paxs	214.29	Joback Method
dvisc	0.0009378	Paxs	241.58	Joback Method
dvisc	0.0006211	Paxs	268.88	Joback Method
dvisc	0.0004438	Paxs	296.18	Joback Method
dvisc	0.0003356	Paxs	323.47	Joback Method
dvisc	0.0002651	Paxs	350.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36215073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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