

Butane, 1-chloro-4-methoxy-

Other names:	Ether, 4-chlorobutyl methyl 1-Chloro-4-methoxybutane
Inchi:	InChI=1S/C5H11ClO/c1-7-5-3-2-4-6/h2-5H2,1H3
InchiKey:	DFLRARJQZRCCKN-UHFFFAOYSA-N
Formula:	C5H11ClO
SMILES:	COCCCCCI
Mol. weight [g/mol]:	122.59
CAS:	17913-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-125.71	kJ/mol	Joback Method
hf	-294.49	kJ/mol	Joback Method
hfus	14.09	kJ/mol	Joback Method
hvap	33.52	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.652		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	847.30		NIST Webbook
rinpol	840.30		NIST Webbook
tb	373.65	K	Joback Method
tc	546.90	K	Joback Method
tf	198.26	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.70	J/mol×K	373.65	Joback Method
cpg	213.61	J/mol×K	518.02	Joback Method
cpg	205.94	J/mol×K	489.15	Joback Method
cpg	198.02	J/mol×K	460.27	Joback Method
cpg	189.84	J/mol×K	431.40	Joback Method

cpg	181.40	J/mol×K	402.52	Joback Method
cpg	221.03	J/mol×K	546.90	Joback Method
dvisc	0.0002660	Pa×s	373.65	Joback Method
dvisc	0.0003395	Pa×s	344.42	Joback Method
dvisc	0.0004535	Pa×s	315.19	Joback Method
dvisc	0.0006426	Pa×s	285.95	Joback Method
dvisc	0.0009858	Pa×s	256.72	Joback Method
dvisc	0.0016880	Pa×s	227.49	Joback Method
dvisc	0.0033874	Pa×s	198.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17913187&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

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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