1-Butanol, 3-methoxy-

Other names:	3-Methoxy-1-butanol
	3-Methoxybutanol
	3-methoxybutan-1-ol
	Methoxybutanol
Inchi:	InChI=1S/C5H12O2/c1-5(7-2)3-4-6/h5-6H,3-4H2,1-2H3
InchiKey:	JSGVZVOGOQILFM-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	COC(C)CCO
Mol. weight [g/mol]:	104.15
CAS:	2517-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-253.04	kJ/mol	Joback Method
hf	-436.26	kJ/mol	Joback Method
hfus	10.46	kJ/mol	Joback Method
hvap	45.42	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	0.404		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	814.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	782.00		NIST Webbook
tb	433.00 ± 2.00	K	NIST Webbook
tc	593.40	K	Joback Method
tf	214.16	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.34	J/mol×K	427.96	Joback Method
cpg	231.03	J/mol×K	565.83	Joback Method

cpg	223.60	J/mol×K	538.25	Joback Method
cpg	215.92	J/mol×K	510.68	Joback Method
cpg	207.98	J/mol×K	483.11	Joback Method
cpg	199.79	J/mol×K	455.53	Joback Method
cpg	238.21	J/mol×K	593.40	Joback Method
dvisc	0.0002180	Pa×s	427.96	Joback Method
dvisc	0.0003835	Pa×s	392.33	Joback Method
dvisc	0.0007551	Pa×s	356.69	Joback Method
dvisc	0.0017280	Pa×s	321.06	Joback Method
dvisc	0.0048625	Pa×s	285.43	Joback Method
dvisc	0.0183815	Pa×s	249.79	Joback Method
dvisc	0.1081645	Pa×s	214.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59735e+01
Coeff. B	-4.22716e+03
Coeff. C	-6.07320e+01
Temperature range (K), min.	330.22
Temperature range (K), max.	457.20

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=C2517433&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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