1-Butanol, 3-methyl-, formate

Other names:	3-Methylbutyl formate
	Formic acid, 3-methylbutyl ester
	Formic acid, isopentyl ester
	ISOAMYL FORMATE
	ISOAMYL METHANOATE
	ISOPENTYL ESTER FORMIC ACID
	Isopentyl alcohol, formate
	Isopentyl formate
	Isopentyl methanoate
	UN 1109
Inchi:	InChI=1S/C6H12O2/c1-6(2)3-4-8-5-7/h5-6H,3-4H2,1-2H3
InchiKey:	XKYICAQFSCFURC-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC(C)CCOC=O
Mol. weight [g/mol]:	116.16
CAS:	110-45-2

Physical Properties

Property code	Value	Unit	Source
gf	-207.32	kJ/mol	Joback Method
hf	-390.25	kJ/mol	Joback Method
hfus	11.25	kJ/mol	Joback Method
hvap	37.69	kJ/mol	Joback Method
log10ws	-1.52		Estimated Solubility Method
log10ws	-1.52		Aqueous Solubility Prediction Method
logp	1.205		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	775.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	792.90		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	792.00		NIST Webbook

rinpol	775.00		NIST Webbook
rinpol	794.40		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	777.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1058.00		NIST Webbook
tb	396.70	K	KDB
tc	578.00	K	KDB
tf	179.90	K	Aqueous Solubility Prediction Method
tf	179.60	K	KDB
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.69	J/mol×K	407.32	Joback Method
cpg	211.53	J/mol×K	436.76	Joback Method
cpg	221.04	J/mol×K	466.20	Joback Method
cpg	230.24	J/mol×K	495.64	Joback Method
cpg	239.12	J/mol×K	525.08	Joback Method
cpg	247.68	J/mol×K	554.53	Joback Method
cpg	255.92	J/mol×K	583.97	Joback Method
dvisc	0.0022883	Pa×s	240.06	Joback Method
dvisc	0.0052383	Pa×s	206.61	Joback Method
dvisc	0.0012241	Pa×s	273.51	Joback Method
dvisc	0.0007505	Pa×s	306.97	Joback Method
dvisc	0.0005066	Pa×s	340.42	Joback Method
dvisc	0.0003668	Pa×s	373.87	Joback Method

dvisc	0.0002801	Pa×s	407.32	Joback Method
hvapt	38.90	kJ/mol	326.00	NIST Webbook
rhol	882.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55208e+01
Coeff. B	-3.76586e+03
Coeff. C	-5.15850e+01
Temperature range (K), min.	298.80
Temperature range (K), max.	420.45

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.41103e+01
Coeff. B	-4.59151e+03
Coeff. C	3.57105e-01
Coeff. D	-2.86942e-07
Temperature range (K), min.	255.15
Temperature range (K), max.	396.15

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1084.mol

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1084

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C110452&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume