Butanoic acid, 3-methyl-, butyl ester

Other names:	1-Butyl isovalerate
	3-Methylbutyric acid butyl ester
	Butyl 3-methylbutyrate
	Butyl isopentanoate
	Butyl isovalerate
	Butyl isovalerianate
	Isovaleric acid, butyl ester
	NSC 6187
	butyl 3-methylbutanoate
	n-Butyl 3-methylbutanoate
	n-Butyl isopentanoate
	n-Butyl isovalerate
Inchi:	InChI=1S/C9H18O2/c1-4-5-6-11-9(10)7-8(2)3/h8H,4-7H2,1-3H3
InchiKey:	AYWJSCLAAPJZEF-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCOC(=O)CC(C)C
Mol. weight [g/mol]:	158.24
CAS:	109-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1030.00		NIST Webbook

rinpol	1021.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1042.00	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1030.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	1035.00	NIST Webbook
ripol	1259.00	NIST Webbook
ripol	1278.00	NIST Webbook
ripol	1250.00	NIST Webbook
ripol	1278.00	NIST Webbook
ripol	1303.00	NIST Webbook
ripol	1270.00	NIST Webbook
ripol	1264.00	NIST Webbook
ripol	1246.00	NIST Webbook
ripol	1271.00	NIST Webbook
ripol	1250.00	NIST Webbook
ripol	1259.00	NIST Webbook
ripol	1295.00	NIST Webbook
ripol	1252.00	NIST Webbook
ripol	1271.00	NIST Webbook
ripol	1242.00	NIST Webbook

ripol	1259.00		NIST Webbook
ripol	1259.00		NIST Webbook
ripol	1259.00		NIST Webbook
tb	175.70 ± 0.30	K	NIST Webbook
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
dvisc	0.0047844	Pa×s	248.35	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43933e+01
Coeff. B	-3.81960e+03
Coeff. C	-6.57360e+01
Temperature range (K), min.	336.52
Temperature range (K), max.	486.31

Sources

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
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=C109193&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume