Butanoic acid, 3-methyl-, 3-methylbutyl ester

Other names:	3-Methylbutyl 3-methylbutyrate
	3-Methylbutyl isovalerate
	3-methylbutyl 3-methylbutanoate
	Apple essence
	Apple oil
	ISOAMYL ISOVALERATE
	ISOAMYL VALERIANATE
	ISOPENTYL 3-METHYLBUTYRATE
	Isoamyl 3-methylbutanoate
	Isoamyl 3-methylbutyrate
	Isopentyl 3-methylbutanoate
	Isopentyl alcohol, isovalerate
	Isopentyl isopentanoate
	Isopentyl isovalerate
	Isovaleric acid, 3-methylbutyl ester
	Isovaleric acid, isopentyl ester
	NSC 6565
	Solusterol
	iso-Amyl isovalerate
Inchi:	InChI=1S/C10H20O2/c1-8(2)5-6-12-10(11)7-9(3)4/h8-9H,5-7H2,1-4H3
InchiKey:	XINCECQTMHSORG-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CC(C)CCOC(=O)CC(C)C
Mol. weight [g/mol]:	172.26
CAS:	659-70-1

Physical Properties

Property code	Value	Unit	Source
gf	-205.48	kJ/mol	Joback Method
hf	-505.09	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1070.00		NIST Webbook

rinpol	1103.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1106.40	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1090.70	NIST Webbook
rinpol	1090.70	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1103.00	NIST Webbook
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rinpol	1103.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1105.00	NIST Webbook

rinpol	1103.00	NIST Webbook
rinpol	1081.00	NIST Webbook
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rinpol	1104.00	NIST Webbook
rinpol	1104.00	NIST Webbook
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rinpol	1109.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1107.50	NIST Webbook
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rinpol	1103.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1102.00	NIST Webbook
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ripol	1294.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1294.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1280.00		NIST Webbook
tb	463.60	K	NIST Webbook
tb	465.85 ± 0.30	K	NIST Webbook
tb	466.70 ± 0.50	K	NIST Webbook
tb	467.15 ± 1.50	K	NIST Webbook
tc	682.96	K	Joback Method
tf	244.62	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.51	J/mol×K	503.61	Joback Method
cpg	383.39	J/mol×K	533.50	Joback Method
cpg	397.67	J/mol×K	563.39	Joback Method
cpg	411.38	J/mol×K	593.28	Joback Method
cpg	424.51	J/mol×K	623.18	Joback Method
cpg	437.08	J/mol×K	653.07	Joback Method
cpg	449.08	J/mol×K	682.96	Joback Method
dvisc	0.0024917	Pa×s	287.79	Joback Method
dvisc	0.0070487	Pa×s	244.62	Joback Method
dvisc	0.0011553	Pa×s	330.95	Joback Method
dvisc	0.0006396	Pa×s	374.12	Joback Method
dvisc	0.0004002	Pa×s	417.28	Joback Method
dvisc	0.0002734	Pa×s	460.44	Joback Method
dvisc	0.0001994	Pa×s	503.61	Joback Method
hvapt	46.40	kJ/mol	410.00	NIST Webbook
hvapt	47.20	kJ/mol	383.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.97023e+01
Coeff. B	-6.63821e+03
Coeff. C	-3.46649e+00
Coeff. D	1.97306e-06
Temperature range (K), min.	215.00
Temperature range (K), max.	637.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1121.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C659701&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1121
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
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

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