Propanoic acid, 2-methyl-, 3-methylbutyl ester

Other names:	3-methyl-1-butyl isobutyrate
	3-methylbutyl 2-methylpropanoate
	3-methylbutyl isobutyrate
	Isoamyl 2-methylpropanoate
	Isoamyl isobutanoate
	Isopentyl alcohol, isobutyrate
	Isopentyl isobutanoate
	iso-Amyl iso-butyrate
	isoamyl isobutyrate
	isobutyric acid, isopentyl ester
	isopentyl isobutyrate
Inchi:	InChI=1S/C9H18O2/c1-7(2)5-6-11-9(10)8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	VFTGLSWXJMRZNB-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CC(C)CCOC(=O)C(C)C
Mol. weight [g/mol]:	158.24
CAS:	2050-01-3

Physical Properties

Property code	Value	Unit	Source
gf	-213.90	kJ/mol	Joback Method
hf	-484.45	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.232		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1017.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1014.00		NIST Webbook

rinpol	1014.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1013.40		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1018.30		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	997.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1214.00		NIST Webbook
tb	442.95 ± 0.30	K	NIST Webbook
tb	442.10 ± 0.50	K	NIST Webbook
tc	661.81	K	Joback Method
tf	233.35	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.73	J/mol×K	631.63	Joback Method
cpg	375.88	J/mol×K	601.45	Joback Method
cpg	363.51	J/mol×K	571.27	Joback Method
cpg	350.61	J/mol×K	541.09	Joback Method
cpg	337.19	J/mol×K	510.91	Joback Method
cpg	323.22	J/mol×K	480.73	Joback Method
cpg	399.06	J/mol×K	661.81	Joback Method
dvisc	0.0073761	Pa×s	233.35	Joback Method
dvisc	0.0002156	Pa×s	480.73	Joback Method
dvisc	0.0002948	Pa×s	439.50	Joback Method
dvisc	0.0004299	Pa×s	398.27	Joback Method
dvisc	0.0006840	Pa×s	357.04	Joback Method
dvisc	0.0012286	Pa×s	315.81	Joback Method
dvisc	0.0026314	Pa×s	274.58	Joback Method
hvapt	51.70	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography
hvapt	47.40	kJ/mol	364.50	NIST Webbook

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography: https://www.doi.org/10.1016/j.jct.2015.02.015

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=C2050013&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
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