Isobutyl isovalerate

Other names:	Butanoic acid, 3-methyl-, 2-methylpropyl ester
	Isovaleric acid, isobutyl ester
	2-Methylpropyl isovalerate
	2-Methylpropyl 3-methylbutyrate
	Isobutyl 3-methylpropanoate
	Isobutyl isopentanoate
	Isobutyl 3-methylbutanoate
	2-Methylpropyl 3-methylbutanoate
	NSC 6993
Inchi:	InChI=1S/C9H18O2/c1-7(2)5-9(10)11-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	KEBDNKNVCHQIJU-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CC(C)COC(=O)CC(C)C
Mol. weight [g/mol]:	158.24
CAS:	589-59-3

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	989.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1012.70		NIST Webbook
rinpol	1018.00		NIST Webbook

rinpol	990.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1004.00		NIST Webbook
ripol	1175.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1198.00		NIST Webbook
ripol	1184.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1198.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1190.00		NIST Webbook
tb	444.35 ± 0.30	K	NIST Webbook
tb	441.90 ± 0.50	K	NIST Webbook
tb	168.10 ± 0.30	K	NIST Webbook
tc	621.40 ± 6.00	K	NIST Webbook
tf	233.35	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.22	J/mol×K	480.73	Joback Method
cpg	337.19	J/mol×K	510.91	Joback Method
cpg	350.61	J/mol×K	541.09	Joback Method
cpg	363.51	J/mol×K	571.27	Joback Method
cpg	375.88	J/mol×K	601.45	Joback Method
cpg	387.73	J/mol×K	631.63	Joback Method
cpg	399.06	J/mol×K	661.81	Joback Method
dvisc	0.0073761	Pa×s	233.35	Joback Method
dvisc	0.0026314	Pa×s	274.58	Joback Method
dvisc	0.0012286	Pa×s	315.81	Joback Method
dvisc	0.0006840	Pa×s	357.04	Joback Method
dvisc	0.0004299	Pa×s	398.27	Joback Method
dvisc	0.0002948	Pa×s	439.50	Joback Method
dvisc	0.0002156	Pa×s	480.73	Joback Method
hvapt	47.30	kJ/mol	365.50	NIST Webbook

Sources

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=C589593&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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