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

Other names:	2-Methylbutyl 2-methylpropanoate
	2-Methylbutyl isobutanoate
	2-Methylbutyl isobutyrate
	2-Metylbutyl Isobutyrate
	Isobutyric acid, 2-methylbutyl ester
Inchi:	InChI=1S/C9H18O2/c1-5-8(4)6-11-9(10)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey:	DUAXUBMIVRZGCO-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCC(C)COC(=O)C(C)C
Mol. weight [g/mol]:	158.24
CAS:	2445-69-4

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	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1021.50		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1016.70		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1014.00		NIST Webbook

rinpol	1014.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1021.50		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1203.00		NIST Webbook
tb	480.73	K	Joback Method
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	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36055e+01
Coeff. B	-3.53677e+03
Coeff. C	-6.29560e+01
Temperature range (K), min.	328.52
Temperature range (K), max.	489.38

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2445694&Units=SI
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

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