Butanoic acid, 3-methyl-, propyl ester

Other names:	3-Methylbutanoic acid, propyl ester
	3-methyl propyl butanoate
	Isovaleric acid, propyl ester
	Propyl 3-methylbutanoate
	Propyl 3-methylbutyrate
	Propyl isopentanoate
	Propyl isovalerate
	n-Propyl iso-valerate
Inchi:	InChI=1S/C8H16O2/c1-4-5-10-8(9)6-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	LSJMDWFAADPNAX-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCOC(=O)CC(C)C
Mol. weight [g/mol]:	144.21
CAS:	557-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-219.88	kJ/mol	Joback Method
hf	-458.53	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	912.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	949.00		NIST Webbook

rinpol	924.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	949.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1144.00		NIST Webbook
tb	428.95 ± 0.30	K	NIST Webbook
tb	429.00 ± 0.50	K	NIST Webbook
tb	154.60 ± 0.30	K	NIST Webbook
tc	609.08 ± 6.00	K	NIST Webbook
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.57	J/mol×K	637.16	Joback Method
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method

dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
hvapt	44.30	kJ/mol	355.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50271e+01
Coeff. B	-3.83415e+03
Coeff. C	-6.05930e+01
Temperature range (K), min.	320.72
Temperature range (K), max.	455.23

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C557006&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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1101.mol

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