Butanoic acid, 3-methyl-, 1-methylethyl ester

Other names:	Isopropyl 3-methylbutanoate
	Isopropyl isopentanoate
	iso-Propyl iso-valerate
	isopropyl 3-methylbutyrate
Inchi:	InChI=1S/C8H16O2/c1-6(2)5-8(9)10-7(3)4/h6-7H,5H2,1-4H3
InchiKey:	ZOIRKXLFEHOVER-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CC(C)CC(=O)OC(C)C
Mol. weight [g/mol]:	144.21
CAS:	32665-23-9

Physical Properties

Property code	Value	Unit	Source
gf	-222.32	kJ/mol	Joback Method
hf	-463.81	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	41.78	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.984		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	880.00		NIST Webbook
ripol	1083.00		NIST Webbook
ripol	1034.00		NIST Webbook
ripol	1071.00		NIST Webbook

tb	141.80 ± 0.30	K	NIST Webbook
tc	640.65	K	Joback Method
tf	222.08	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.95	J/mol×K	457.85	Joback Method
cpg	292.89	J/mol×K	488.32	Joback Method
cpg	305.35	J/mol×K	518.78	Joback Method
cpg	317.32	J/mol×K	549.25	Joback Method
cpg	328.83	J/mol×K	579.72	Joback Method
cpg	339.86	J/mol×K	610.19	Joback Method
cpg	350.42	J/mol×K	640.65	Joback Method
dvisc	0.0076048	Pa×s	222.08	Joback Method
dvisc	0.0027406	Pa×s	261.38	Joback Method
dvisc	0.0012896	Pa×s	300.67	Joback Method
dvisc	0.0007223	Pa×s	339.97	Joback Method
dvisc	0.0004562	Pa×s	379.26	Joback Method
dvisc	0.0003141	Pa×s	418.56	Joback Method
dvisc	0.0002306	Pa×s	457.85	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32395e+01
Coeff. B	-3.27111e+03
Coeff. C	-5.65620e+01
Temperature range (K), min.	309.12
Temperature range (K), max.	469.16

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32665239&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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