Butanoic acid, 2-methyl-, 1-methylethyl ester

Other names:	Isopropyl 2-methylbutanoate
	2-Propyl 2-methylbutanoate
	Isopropyl 2-methylbutyrate
	1-Methylethyl 2-methylbutanoate
	isopropyl 2-methylbutyrate
Inchi:	InChI=1S/C8H16O2/c1-5-7(4)8(9)10-6(2)3/h6-7H,5H2,1-4H3
InchiKey:	DIRDKDDFAMNBNY-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCC(C)C(=O)OC(C)C
Mol. weight [g/mol]:	144.21
CAS:	66576-71-4

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	960.00		NIST Webbook
ripol	1052.00		NIST Webbook
ripol	1061.00		NIST Webbook
tb	457.85	K	Joback Method
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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66576714&Units=SI

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

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