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

Physical Properties

Property code	Value	Unit	Source
af	0.4503		Cheméo Relay (1.0)
hf	-567.04	kJ/mol	Cheméo Relay (1.0)
hfus	12.22	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.984		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
ripol	1052.00		NIST Webbook
ripol	1061.00		NIST Webbook
tb	382.50	K	Cheméo Relay (1.0)
tc	580.84	K	Cheméo Relay (1.0)
tf	203.14	K	Cheméo Relay (1.0)
vc	0.494	m3/kmol	Cheméo Relay (1.0)

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
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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