BUTYRIC ACID, 2-BROMO-, 1-METHYLETHYL ESTER

Other names: Isopropyl 2-bromobutanoate
Inchi: InChI=1S/C7H13BrO2/c1-4-6(8)7(9)10-5(2)3/h5-6H,4H2,1-3H3
InchiKey: XSRQGXVWFDYHQT-UHFFFAOYSA-N
Formula: C7H13BrO2
SMILES: CCC(Br)C(=O)OC(C)C
Mol. weight [g/mol]: 209.08

Physical Properties

Property code	Value	Unit	Source
hf	-514.74	kJ/mol	Cheméo Relay (1.0)
hfus	14.91	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Cheméo Relay (1.0)
ie	9.90	eV	Cheméo Relay (1.0)
log10ws	-2.29		Cheméo Relay (1.0)
logp	2.111		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1033.00		NIST Webbook
tb	433.24	K	Cheméo Relay (1.0)
tc	627.55	K	Cheméo Relay (1.0)
tf	257.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.34	J/mol×K	501.13	Joback Method
cpg	338.71	J/mol×K	701.72	Joback Method
cpg	329.75	J/mol×K	668.28	Joback Method
cpg	320.30	J/mol×K	634.85	Joback Method
cpg	310.34	J/mol×K	601.42	Joback Method
cpg	299.87	J/mol×K	567.99	Joback Method
cpg	288.87	J/mol×K	534.56	Joback Method
dvisc	0.0007361	Pa×s	385.87	Joback Method
dvisc	0.0002675	Pa×s	501.13	Joback Method

dvisc	0.0003544	Pa×s	462.71	Joback Method
dvisc	0.0004941	Pa×s	424.29	Joback Method
dvisc	0.0047978	Pa×s	270.61	Joback Method
dvisc	0.0011975	Pa×s	347.45	Joback Method
dvisc	0.0021989	Pa×s	309.03	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U131992&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

Legend

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point