Butanoic acid, 2-bromo-3-methyl-, ethyl ester

Other names:	Ethyl «alpha»-bromoisovalerate
	Ethyl 2-bromo-3-methylbutyrate
	Ethyl 2-bromoisovalerate
	«alpha»-Bromoisovaleric acid ethyl ester
	Butyric acid, 2-bromo-3-methyl-, ethyl ester
	Ethyl 2-bromo-3-methylbutanoate
Inchi:	InChI=1S/C7H13BrO2/c1-4-10-7(9)6(8)5(2)3/h5-6H,4H2,1-3H3
InchiKey:	WNFUWONOILPKNX-UHFFFAOYSA-N
Formula:	C7H13BrO2
SMILES:	CCOC(=O)C(Br)C(C)C
Mol. weight [g/mol]:	209.08
CAS:	609-12-1

Physical Properties

Property code	Value	Unit	Source
gf	-216.42	kJ/mol	Joback Method
hf	-416.84	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.969		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	501.13	K	Joback Method
tc	701.72	K	Joback Method
tf	270.61	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.34	J/mol×K	501.13	Joback Method
cpg	288.87	J/mol×K	534.56	Joback Method
cpg	299.87	J/mol×K	567.99	Joback Method

cpg	310.34	J/mol×K	601.42	Joback Method
cpg	320.30	J/mol×K	634.85	Joback Method
cpg	329.75	J/mol×K	668.28	Joback Method
cpg	338.71	J/mol×K	701.72	Joback Method
dvisc	0.0047978	Pa×s	270.61	Joback Method
dvisc	0.0021989	Pa×s	309.03	Joback Method
dvisc	0.0011975	Pa×s	347.45	Joback Method
dvisc	0.0007361	Pa×s	385.87	Joback Method
dvisc	0.0004941	Pa×s	424.29	Joback Method
dvisc	0.0003544	Pa×s	462.71	Joback Method
dvisc	0.0002675	Pa×s	501.13	Joback Method

Sources

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=C609121&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume