iso-Butyl 2-bromopropionate

Other names:	Propanoic acid, 2-bromo-, 2-methylpropyl ester
	2-Bromopropionic acid, 2-methylpropyl ester
	Propanoic acid, 2-bromo, isobutyl ester
	Isobutyl 2-bromopropanoate
Inchi:	InChI=1S/C7H13BrO2/c1-5(2)4-10-7(9)6(3)8/h5-6H,4H2,1-3H3
InchiKey:	MAYJUJUXGCDPPX-UHFFFAOYSA-N
Formula:	C7H13BrO2
SMILES:	CC(C)COC(=O)C(C)Br
Mol. weight [g/mol]:	209.08
CAS:	69122-46-9

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
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1056.00		NIST Webbook
ripol	1438.00		NIST Webbook
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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69122469&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