Isobutyl 3-bromopropanoate

Other names: Propanoic acid, 3-bromo, isobutyl ester
Inchi: InChI=1S/C7H13BrO2/c1-6(2)5-10-7(9)3-4-8/h6H,3-5H2,1-2H3
InchiKey: SMOUSNHACQMSQG-UHFFFAOYSA-N
Formula: C7H13BrO2
SMILES: CC(C)COC(=O)CCBr
Mol. weight [g/mol]: 209.08

Physical Properties

Property code	Value	Unit	Source
gf	-213.98	kJ/mol	Joback Method
hf	-411.56	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.971		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1136.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	501.57	K	Joback Method
tc	697.81	K	Joback Method
tf	285.61	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.07	J/mol×K	501.57	Joback Method
cpg	288.28	J/mol×K	534.28	Joback Method
cpg	298.99	J/mol×K	566.98	Joback Method
cpg	309.20	J/mol×K	599.69	Joback Method
cpg	318.93	J/mol×K	632.40	Joback Method
cpg	328.18	J/mol×K	665.11	Joback Method

cpg	336.97	J/mol×K	697.81	Joback Method
dvisc	0.0034561	Pa×s	285.61	Joback Method
dvisc	0.0018031	Pa×s	321.60	Joback Method
dvisc	0.0010723	Pa×s	357.60	Joback Method
dvisc	0.0007013	Pa×s	393.59	Joback Method
dvisc	0.0004925	Pa×s	429.58	Joback Method
dvisc	0.0003653	Pa×s	465.58	Joback Method
dvisc	0.0002828	Pa×s	501.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30143&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

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