Isopropyl 2-bromopropanoate

Other names: Propanoic acid, 2-bromo, isopropyl ester
Inchi: InChI=1S/C6H11BrO2/c1-4(2)9-6(8)5(3)7/h4-5H,1-3H3
InchiKey: ODCLWDCSAGRHKS-UHFFFAOYSA-N
Formula: C6H11BrO2
SMILES: CC(C)OC(=O)C(C)Br
Mol. weight [g/mol]: 195.05

Physical Properties

Property code	Value	Unit	Source
gf	-224.84	kJ/mol	Joback Method
hf	-396.20	kJ/mol	Joback Method
hfus	12.32	kJ/mol	Joback Method
hvap	43.77	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.721		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	945.00		NIST Webbook
ripol	1316.00		NIST Webbook
tb	478.25	K	Joback Method
tc	681.58	K	Joback Method
tf	259.34	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.75	J/mol×K	478.25	Joback Method
cpg	282.95	J/mol×K	647.69	Joback Method
cpg	274.43	J/mol×K	613.80	Joback Method
cpg	265.45	J/mol×K	579.91	Joback Method
cpg	256.02	J/mol×K	546.03	Joback Method

cpg	246.12	J/mol×K	512.14	Joback Method
cpg	291.03	J/mol×K	681.58	Joback Method
dvisc	0.0002941	Pa×s	478.25	Joback Method
dvisc	0.0003880	Pa×s	441.76	Joback Method
dvisc	0.0005380	Pa×s	405.28	Joback Method
dvisc	0.0007958	Pa×s	368.80	Joback Method
dvisc	0.0012829	Pa×s	332.31	Joback Method
dvisc	0.0023268	Pa×s	295.83	Joback Method
dvisc	0.0049896	Pa×s	259.34	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R23223&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

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