2-Bromopropionic acid, 3-methylbutyl ester

Other names:	Propanoic acid, 2-bromo, 3-methylbutyl ester
	Propanoic acid, 2-bromo, isopentyl ester
	Isopentyl 2-bromopropanoate
Inchi:	InChI=1S/C8H15BrO2/c1-6(2)4-5-11-8(10)7(3)9/h6-7H,4-5H2,1-3H3
InchiKey:	GVDWMKVPTHSZKA-UHFFFAOYSA-N
Formula:	C8H15BrO2
SMILES:	CC(C)CCOC(=O)C(C)Br
Mol. weight [g/mol]:	223.11
CAS:	86711-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-208.00	kJ/mol	Joback Method
hf	-437.48	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.359		Crippen Method
mcvol	148.520	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1163.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	524.01	K	Joback Method
tc	721.87	K	Joback Method
tf	281.88	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.93	J/mol×K	524.01	Joback Method
cpg	333.49	J/mol×K	556.99	Joback Method
cpg	345.46	J/mol×K	589.96	Joback Method

cpg	356.85	J/mol×K	622.94	Joback Method
cpg	367.67	J/mol×K	655.92	Joback Method
cpg	377.94	J/mol×K	688.90	Joback Method
cpg	387.67	J/mol×K	721.87	Joback Method
dvisc	0.0045596	Pa×s	281.88	Joback Method
dvisc	0.0020562	Pa×s	322.24	Joback Method
dvisc	0.0011072	Pa×s	362.59	Joback Method
dvisc	0.0006748	Pa×s	402.94	Joback Method
dvisc	0.0004501	Pa×s	443.30	Joback Method
dvisc	0.0003212	Pa×s	483.65	Joback Method
dvisc	0.0002415	Pa×s	524.01	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86711742&Units=SI

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