Bromoacetic acid, 3-methylbutyl ester

Other names:	Acetic acid, bromo, 3-methylbutyl ester
	Isopentyl bromoacetate
Inchi:	InChI=1S/C7H13BrO2/c1-6(2)3-4-10-7(9)5-8/h6H,3-5H2,1-2H3
InchiKey:	QHIYUCHMHDAPAT-UHFFFAOYSA-N
Formula:	C7H13BrO2
SMILES:	CC(C)CCOC(=O)CBr
Mol. weight [g/mol]:	209.08
CAS:	83004-92-6

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	1125.00		NIST Webbook
rinpol	1127.90		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1127.90		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1595.00		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

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=C83004926&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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