Butanoic acid, 3-methyl, 2-bromoethyl ester

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

Physical Properties

Property code	Value	Unit	Source
hf	-499.04	kJ/mol	Cheméo Relay (1.0)
hfus	20.02	kJ/mol	Joback Method
hvap	53.33	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
logp	1.971		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
tb	442.18	K	Cheméo Relay (1.0)
tc	658.02	K	Cheméo Relay (1.0)
tf	228.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.44	J/mol×K	483.70	Joback Method
cpg	284.96	J/mol×K	515.91	Joback Method
cpg	295.94	J/mol×K	548.11	Joback Method
cpg	306.38	J/mol×K	580.32	Joback Method
cpg	316.30	J/mol×K	612.53	Joback Method
cpg	325.71	J/mol×K	644.74	Joback Method
cpg	334.61	J/mol×K	676.94	Joback Method
dvisc	0.0058825	Pa×s	255.78	Joback Method
dvisc	0.0025136	Pa×s	293.77	Joback Method
dvisc	0.0013049	Pa×s	331.75	Joback Method

dvisc	0.0007752	Pa×s	369.74	Joback Method
dvisc	0.0005074	Pa×s	407.73	Joback Method
dvisc	0.0003570	Pa×s	445.71	Joback Method
dvisc	0.0002654	Pa×s	483.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R19836&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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