

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
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
mvol	134.430	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
tb	501.57	K	Joback Method
tc	697.81	K	Joback Method
tf	285.61	K	Joback Method
vc	0.507	m ³ /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	Paxs	285.61	Joback Method
dvisc	0.0018031	Paxs	321.60	Joback Method
dvisc	0.0010723	Paxs	357.60	Joback Method
dvisc	0.0007013	Paxs	393.59	Joback Method
dvisc	0.0004925	Paxs	429.58	Joback Method
dvisc	0.0003653	Paxs	465.58	Joback Method
dvisc	0.0002828	Paxs	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=R19836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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