Ethyl 4-bromobutyrate

Other names:	BrCH2CH2CH2C(O)OC2H5
	Ethyl «gamma»-bromobutyrate
	Butanoic acid, 4-bromo-, ethyl ester
	4-Bromobutanoic acid, ethyl ester
Inchi:	InChI=1S/C6H11BrO2/c1-2-9-6(8)4-3-5-7/h2-5H2,1H3
InchiKey:	XBPOBCXHALHJFP-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CCOC(=O)CCCBr
Mol. weight [g/mol]:	195.05
CAS:	2969-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-219.96	kJ/mol	Joback Method
hf	-385.64	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.725		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	479.13	K	Joback Method
tc	673.53	K	Joback Method
tf	289.34	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.29	J/mol×K	479.13	Joback Method
cpg	245.05	J/mol×K	511.53	Joback Method
cpg	254.40	J/mol×K	543.93	Joback Method
cpg	263.33	J/mol×K	576.33	Joback Method
cpg	271.87	J/mol×K	608.73	Joback Method

cpg	280.00	J/mol×K	641.13	Joback Method
cpg	287.75	J/mol×K	673.53	Joback Method
dvisc	0.0026449	Pa×s	289.34	Joback Method
dvisc	0.0015715	Pa×s	320.97	Joback Method
dvisc	0.0010251	Pa×s	352.60	Joback Method
dvisc	0.0007175	Pa×s	384.24	Joback Method
dvisc	0.0005301	Pa×s	415.87	Joback Method
dvisc	0.0004089	Pa×s	447.50	Joback Method
dvisc	0.0003263	Pa×s	479.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.20	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2969815&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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume