2-Butenoic acid, 4-bromo-, ethyl ester, (E)-

Other names:	Ethyl (E)-4-bromo-2-butenoate
	Ethyl «gamma»-bromocrotonate
	Ethyl 4-bromocrotonate
Inchi:	InChI=1S/C6H9BrO2/c1-2-9-6(8)4-3-5-7/h3-4H,2,5H2,1H3/b4-3+
InchiKey:	FHGRPBSDPBRTLS-ONEGZZNKSA-N
Formula:	C6H9BrO2
SMILES:	CCOC(=O)C=CCBr
Mol. weight [g/mol]:	193.04
CAS:	37746-78-4

Physical Properties

Property code	Value	Unit	Source
gf	-139.74	kJ/mol	Joback Method
hf	-268.42	kJ/mol	Joback Method
hfus	19.57	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.501		Crippen Method
mcvol	116.040	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
tb	483.29	K	Joback Method
tc	687.04	K	Joback Method
tf	284.26	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.83	J/mol×K	483.29	Joback Method
cpg	227.03	J/mol×K	517.25	Joback Method
cpg	235.76	J/mol×K	551.21	Joback Method
cpg	244.02	J/mol×K	585.16	Joback Method
cpg	251.85	J/mol×K	619.12	Joback Method
cpg	259.25	J/mol×K	653.08	Joback Method

cpg	266.25	J/mol×K	687.04	Joback Method
dvisc	0.0024279	Pa×s	284.26	Joback Method
dvisc	0.0013964	Pa×s	317.43	Joback Method
dvisc	0.0008917	Pa×s	350.60	Joback Method
dvisc	0.0006154	Pa×s	383.77	Joback Method
dvisc	0.0004505	Pa×s	416.95	Joback Method
dvisc	0.0003453	Pa×s	450.12	Joback Method
dvisc	0.0002745	Pa×s	483.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.70	K	1.60	NIST Webbook
tbrp	376.50 ± 0.50	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37746784&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