2-Butenoic acid, 4-bromo-, methyl ester

Other names:	4-Bromo-2-butenoic acid methyl ester
	Crotonic acid, 4-bromo-, methyl ester
	Methyl 4-bromo-2-butenoate
	Methyl bromocrotonate
	Methyl «gamma»-bromocrotonate
	Methyl 4-bromocrotonate
Inchi:	InChI=1S/C5H7BrO2/c1-8-5(7)3-2-4-6/h2-3H,4H2,1H3/b3-2+
InchiKey:	RWIKCBHOVNDESJ-NSCUHMNNSA-N
Formula:	C5H7BrO2
SMILES:	COC(=O)C=CCBr
Mol. weight [g/mol]:	179.01
CAS:	1117-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-148.16	kJ/mol	Joback Method
hf	-247.78	kJ/mol	Joback Method
hfus	16.98	kJ/mol	Joback Method
hvap	42.27	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.110		Crippen Method
mcvol	101.950	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	460.41	K	Joback Method
tc	666.92	K	Joback Method
tf	272.99	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.89	J/mol×K	460.41	Joback Method
cpg	186.79	J/mol×K	494.83	Joback Method
cpg	194.27	J/mol×K	529.25	Joback Method

cpg	201.36	J/mol×K	563.66	Joback Method
cpg	208.06	J/mol×K	598.08	Joback Method
cpg	214.39	J/mol×K	632.50	Joback Method
cpg	220.37	J/mol×K	666.92	Joback Method
dvisc	0.0024211	Pa×s	272.99	Joback Method
dvisc	0.0014243	Pa×s	304.23	Joback Method
dvisc	0.0009249	Pa×s	335.46	Joback Method
dvisc	0.0006465	Pa×s	366.70	Joback Method
dvisc	0.0004780	Pa×s	397.94	Joback Method
dvisc	0.0003693	Pa×s	429.17	Joback Method
dvisc	0.0002955	Pa×s	460.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	1.70	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1117711&Units=SI

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