Propanoic acid, 3-bromo-2-oxo-, ethyl ester

Other names:	Pyruvic acid, bromo-, ethyl ester
	«beta»-Bromopyruvic acid ethyl ester
	Ethyl bromopyruvate
	Bromopyruvic acid ethyl ester
	Ethyl 3-bromopyruvate
Inchi:	InChI=1S/C5H7BrO3/c1-2-9-5(8)4(7)3-6/h2-3H2,1H3
InchiKey:	VICYTAYPKBLQFB-UHFFFAOYSA-N
Formula:	C5H7BrO3
SMILES:	CCOC(=O)C(=O)CBr
Mol. weight [g/mol]:	195.01
CAS:	70-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-357.30	kJ/mol	Joback Method
hf	-477.58	kJ/mol	Joback Method
hfus	18.38	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	0.513		Crippen Method
mcvol	107.820	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	510.12	K	Joback Method
tc	716.96	K	Joback Method
tf	328.00	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.40	J/mol×K	510.12	Joback Method
cpg	241.54	J/mol×K	682.49	Joback Method
cpg	235.24	J/mol×K	648.01	Joback Method
cpg	228.58	J/mol×K	613.54	Joback Method

cpg	221.56	J/mol×K	579.07	Joback Method
cpg	214.16	J/mol×K	544.59	Joback Method
cpg	247.48	J/mol×K	716.96	Joback Method
dvisc	0.0003799	Pa×s	510.12	Joback Method
dvisc	0.0004679	Pa×s	479.77	Joback Method
dvisc	0.0005928	Pa×s	449.41	Joback Method
dvisc	0.0007772	Pa×s	419.06	Joback Method
dvisc	0.0010630	Pa×s	388.71	Joback Method
dvisc	0.0015331	Pa×s	358.35	Joback Method
dvisc	0.0023661	Pa×s	328.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	1.30	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=C70235&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