Propanoic acid, 3-bromo-, ethyl ester

Other names:	Propionic acid, 3-bromo-, ethyl ester
	Ethyl «beta»-bromopropionate
	Ethyl 3-bromopropanoate
	Ethyl 3-bromopropionate
	3-Bromopropionic acid ethyl ester
	«beta»-Bromopropionic acid ethyl ester
Inchi:	InChI=1S/C5H9BrO2/c1-2-8-5(7)3-4-6/h2-4H2,1H3
InchiKey:	FQTIYMRSUOADDK-UHFFFAOYSA-N
Formula:	C5H9BrO2
SMILES:	CCOC(=O)CCBr
Mol. weight [g/mol]:	181.03
CAS:	539-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-228.38	kJ/mol	Joback Method
hf	-365.00	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.334		Crippen Method
mcvol	106.250	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1007.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook
tb	456.25	K	Joback Method
tc	652.96	K	Joback Method
tf	278.07	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.91	J/mol×K	456.25	Joback Method
cpg	204.39	J/mol×K	489.03	Joback Method
cpg	212.52	J/mol×K	521.82	Joback Method
cpg	220.31	J/mol×K	554.60	Joback Method
cpg	227.76	J/mol×K	587.39	Joback Method
cpg	234.86	J/mol×K	620.17	Joback Method
cpg	241.64	J/mol×K	652.96	Joback Method
dvisc	0.0026445	Pa×s	278.07	Joback Method
dvisc	0.0016076	Pa×s	307.77	Joback Method
dvisc	0.0010668	Pa×s	337.46	Joback Method
dvisc	0.0007565	Pa×s	367.16	Joback Method
dvisc	0.0005647	Pa×s	396.86	Joback Method
dvisc	0.0004391	Pa×s	426.55	Joback Method
dvisc	0.0003528	Pa×s	456.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.70	K	6.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C539742&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume