Acetic acid, bromo-, methyl ester

Other names:	Bromoacetic acid methyl ester
	Methyl «alpha»-bromoacetate
	Methyl bromoacetate
	Methyl 2-bromoacetate
	Methyl monobromoacetate
	Methylester kyseliny bromoctove
	UN 2643
	Acetic acid, 2-bromo-, methyl ester
	NSC 2642
Inchi:	InChI=1S/C3H5BrO2/c1-6-3(5)2-4/h2H2,1H3
InchiKey:	YDCHPLOFQATIDS-UHFFFAOYSA-N
Formula:	C3H5BrO2
SMILES:	COC(=O)CBr
Mol. weight [g/mol]:	152.97
CAS:	96-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-245.22	kJ/mol	Joback Method
hf	-323.72	kJ/mol	Joback Method
hfus	11.60	kJ/mol	Joback Method
hvap	37.86	kJ/mol	Joback Method
ie	10.37 ± 0.05	eV	NIST Webbook
log10ws	-0.37		Crippen Method
logp	0.554		Crippen Method
mcvol	78.070	ml/mol	McGowan Method
pc	5168.28	kPa	Joback Method
rinpol	800.20		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	793.00		NIST Webbook
tb	417.00	K	NIST Webbook
tc	611.45	K	Joback Method
tf	255.53	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.98	J/mol×K	410.49	Joback Method
cpg	129.47	J/mol×K	443.98	Joback Method
cpg	134.75	J/mol×K	477.48	Joback Method
cpg	139.83	J/mol×K	510.97	Joback Method
cpg	144.72	J/mol×K	544.46	Joback Method
cpg	149.40	J/mol×K	577.96	Joback Method
cpg	153.88	J/mol×K	611.45	Joback Method
dvisc	0.0025095	Pa×s	255.53	Joback Method
dvisc	0.0016040	Pa×s	281.36	Joback Method
dvisc	0.0011054	Pa×s	307.18	Joback Method
dvisc	0.0008070	Pa×s	333.01	Joback Method
dvisc	0.0006165	Pa×s	358.84	Joback Method
dvisc	0.0004883	Pa×s	384.66	Joback Method
dvisc	0.0003983	Pa×s	410.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	324.70	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=C96322&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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume