Bromoacetic acid, isopropyl ester

Other names:	BrCH2C(O)OCH(CH3)2
	Acetic acid, bromo-, 1-methylethyl ester
	Bromoacetic acid, isopropyl ester
	Acetic acid, 2-bromo-, 1-methylethyl ester
	Isopropyl «alpha»-bromoacetate
Inchi:	InChI=1S/C5H9BrO2/c1-4(2)8-5(7)3-6/h4H,3H2,1-2H3
InchiKey:	JCWLEWKPXYZHGQ-UHFFFAOYSA-N
Formula:	C5H9BrO2
SMILES:	CC(C)OC(=O)CBr
Mol. weight [g/mol]:	181.03

Physical Properties

Property code	Value	Unit	Source
hf	-471.08	kJ/mol	Cheméo Relay (1.0)
hfus	13.25	kJ/mol	Joback Method
hvap	44.80	kJ/mol	Cheméo Relay (1.0)
ie	10.10	eV	Cheméo Relay (1.0)
log10ws	-1.50		Cheméo Relay (1.0)
logp	1.333		Crippen Method
mcvol	106.250	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	949.00		NIST Webbook
rinpol	916.20		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	906.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1365.00		NIST Webbook
tb	418.69	K	Cheméo Relay (1.0)
tc	611.98	K	Cheméo Relay (1.0)
tf	261.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.09	J/mol×K	455.81	Joback Method
cpg	204.86	J/mol×K	489.36	Joback Method
cpg	213.25	J/mol×K	522.90	Joback Method
cpg	221.27	J/mol×K	556.45	Joback Method
cpg	228.93	J/mol×K	590.00	Joback Method
cpg	236.22	J/mol×K	623.55	Joback Method
cpg	243.15	J/mol×K	657.09	Joback Method
dvisc	0.0035835	Pa×s	263.07	Joback Method
dvisc	0.0019491	Pa×s	295.19	Joback Method
dvisc	0.0011948	Pa×s	327.32	Joback Method
dvisc	0.0007993	Pa×s	359.44	Joback Method
dvisc	0.0005712	Pa×s	391.56	Joback Method
dvisc	0.0004295	Pa×s	423.69	Joback Method
dvisc	0.0003362	Pa×s	455.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	1.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29921571&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point