Ethane, 2-bromo-1,1-dimethoxy-

Other names:	Acetaldehyde, bromo-, dimethyl acetal
	Bromoacetal
	Bromoacetaldehyde dimethyl acetal
	2,2-Dimethoxybromoethane
	Dimethylbromoacetal
	1-Bromo-2,2-dimethoxyethane
	2-Bromo-1,1-dimethoxyethane
	2-Bromoacetaldehyde dimethyl acetal
	2,2-Dimethoxyethyl bromide
Inchi:	InChI=1S/C4H9BrO2/c1-6-4(3-5)7-2/h4H,3H2,1-2H3
InchiKey:	FUSFWUFSEJXMRQ-UHFFFAOYSA-N
Formula:	C4H9BrO2
SMILES:	COC(CBr)OC
Mol. weight [g/mol]:	169.02
CAS:	7252-83-7

Physical Properties

Property code	Value	Unit	Source
gf	-215.32	kJ/mol	Joback Method
hf	-369.28	kJ/mol	Joback Method
hfus	10.25	kJ/mol	Joback Method
hvap	35.37	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	1.000		Crippen Method
mcvol	96.460	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	422.20	K	NIST Webbook
tc	591.85	K	Joback Method
tf	224.10	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	167.78	J/mol×K	401.48	Joback Method
cpg	175.46	J/mol×K	433.21	Joback Method
cpg	182.95	J/mol×K	464.94	Joback Method
cpg	190.23	J/mol×K	496.66	Joback Method
cpg	197.30	J/mol×K	528.39	Joback Method
cpg	204.14	J/mol×K	560.12	Joback Method
cpg	210.76	J/mol×K	591.85	Joback Method
dvisc	0.0032247	Pa×s	224.10	Joback Method
dvisc	0.0016800	Pa×s	253.66	Joback Method
dvisc	0.0010028	Pa×s	283.23	Joback Method
dvisc	0.0006599	Pa×s	312.79	Joback Method
dvisc	0.0004668	Pa×s	342.35	Joback Method
dvisc	0.0003489	Pa×s	371.92	Joback Method
dvisc	0.0002722	Pa×s	401.48	Joback Method

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=C7252837&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
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume