Ethane, 2-bromo-1,1-diethoxy-

Other names:	Acetaldehyde, bromo-, diethyl acetal
	Bromacetal
	Bromoacetaldehyde diethyl acetal
	Diethyl bromoacetaldehyde acetal
	1-Bromo-2,2-diethoxyethane
	1,1-Diethoxy-2-bromoethane
	2-Bromoacetaldehyde diethyl acetal
	Bromoacetal
	Diethyl bromoacetal
	2-Bromo-1,1-diethoxyethane
	2,2-Diethoxyethyl bromide
	NSC 8036
Inchi:	InChI=1S/C6H13BrO2/c1-3-8-6(5-7)9-4-2/h6H,3-5H2,1-2H3
InchiKey:	LILXDMFJXYAKMK-UHFFFAOYSA-N
Formula:	C6H13BrO2
SMILES:	CCOC(CBr)OCC
Mol. weight [g/mol]:	197.07
CAS:	2032-35-1

Physical Properties

Property code	Value	Unit	Source
gf	-198.48	kJ/mol	Joback Method
hf	-410.56	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	39.82	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.780		Crippen Method
mcvol	124.640	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
tb	447.24	K	Joback Method
tc	634.34	K	Joback Method
tf	246.64	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.32	J/mol×K	447.24	Joback Method
cpg	252.85	J/mol×K	478.42	Joback Method
cpg	263.04	J/mol×K	509.61	Joback Method
cpg	272.87	J/mol×K	540.79	Joback Method
cpg	282.36	J/mol×K	571.97	Joback Method
cpg	291.49	J/mol×K	603.16	Joback Method
cpg	300.26	J/mol×K	634.34	Joback Method
dvisc	0.0032499	Pa×s	246.64	Joback Method
dvisc	0.0016171	Pa×s	280.07	Joback Method
dvisc	0.0009338	Pa×s	313.51	Joback Method
dvisc	0.0005994	Pa×s	346.94	Joback Method
dvisc	0.0004160	Pa×s	380.37	Joback Method
dvisc	0.0003062	Pa×s	413.81	Joback Method
dvisc	0.0002360	Pa×s	447.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.50 ± 0.50	K	2.40	NIST Webbook
tbrp	339.70	K	2.40	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2032351&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

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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume