2-Ethoxyethyl bromide

Other names:	1-Bromo-2-ethoxyethane
	1-Bromo-2-ethoxyethylene
	1-Bromo-3-oxapentane
	1-Ethoxy-2-bromoethane
	2-Bromoethoxyethane
	2-Bromoethyl ethyl ether
	2-Ethoxyethyl bromide
	Ether, 2-bromoethyl ethyl
	NSC 8026
	UN 2340
Inchi:	InChI=1S/C4H9BrO/c1-2-6-4-3-5/h2-4H2,1H3
InchiKey:	MMYKTRPLXXWLBC-UHFFFAOYSA-N
Formula:	C4H9BrO
SMILES:	CCOCCBr
Mol. weight [g/mol]:	153.02

Physical Properties

Property code	Value	Unit	Source
af	0.4223		Cheméo Relay (1.0)
gf	-107.88	kJ/mol	Joback Method
hf	-241.76	kJ/mol	Cheméo Relay (1.0)
hfus	12.59	kJ/mol	Joback Method
hvap	38.65	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	NIST Webbook
ie	9.94	eV	NIST Webbook
log10ws	-0.85		Cheméo Relay (1.0)
logp	1.418		Crippen Method
mcvol	90.590	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	798.40		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	789.40		NIST Webbook
rinpol	798.00		NIST Webbook
tb	398.00 ± 2.00	K	NIST Webbook
tc	567.66	K	Cheméo Relay (1.0)
tf	180.87	K	Cheméo Relay (1.0)
vc	0.317	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.77	J/mol×K	379.50	Joback Method
cpg	155.34	J/mol×K	410.49	Joback Method
cpg	162.65	J/mol×K	441.47	Joback Method
cpg	169.71	J/mol×K	472.46	Joback Method
cpg	176.51	J/mol×K	503.44	Joback Method
cpg	183.06	J/mol×K	534.43	Joback Method
cpg	189.37	J/mol×K	565.42	Joback Method
dvisc	0.0028309	Pa×s	216.87	Joback Method
dvisc	0.0016164	Pa×s	243.97	Joback Method
dvisc	0.0010324	Pa×s	271.08	Joback Method
dvisc	0.0007153	Pa×s	298.19	Joback Method
dvisc	0.0005269	Pa×s	325.29	Joback Method
dvisc	0.0004068	Pa×s	352.39	Joback Method
dvisc	0.0003259	Pa×s	379.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.70	K	100.00	NIST Webbook
tbrp	313.20	K	3.20	NIST Webbook
tbrp	304.00 ± 1.00	K	1.60	NIST Webbook

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C592552&Units=SI

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

Legend

af:	Acentric Factor
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