

Ethane, 1-bromo-2-ethoxy-

Other names:	Ether, 2-bromoethyl ethyl 1-Bromo-2-ethoxyethane 1-Bromo-2-ethoxyethylene 1-Ethoxy-2-bromoethane 2-Bromoethyl ethyl ether 2-Ethoxyethyl bromide 2-Bromoethoxyethane UN 2340 NSC 8026 1-Bromo-3-oxapentane
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
CAS:	592-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-107.88	kJ/mol	Joback Method
hf	-231.78	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	33.34	kJ/mol	Joback Method
ie	9.94	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	1.418		Crippen Method
mcvol	90.590	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpola	798.40		NIST Webbook
rinpola	798.00		NIST Webbook
rinpola	789.40		NIST Webbook
rinpola	798.00		NIST Webbook
tb	398.00 ± 2.00	K	NIST Webbook
tc	565.42	K	Joback Method
tf	216.87	K	Joback Method
vc	0.340	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

NIST Webbook:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
rinpola:	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

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