Benzene, (2-bromoethoxy)-

Other names:	Phenetole, «beta»-bromo-
	«beta»-Bromophenetole
	«beta»-Phenoxyethyl bromide
	(2-Bromoethoxy)benzene
	1-Bromo-2-phenoxyethane
	2-Bromoethyl phenyl ether
	2-Phenoxyethyl bromide
	beta-Phenoxyethyl bromide
	NSC 8055
Inchi:	InChI=1S/C8H9BrO/c9-6-7-10-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	JJFOBACUIRKUPN-UHFFFAOYSA-N
Formula:	C8H9BrO
SMILES:	BrCCOc1ccccc1
Mol. weight [g/mol]:	201.06
CAS:	589-10-6

Physical Properties

Property code	Value	Unit	Source
gf	38.21	kJ/mol	Joback Method
hf	-77.81	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	44.52	kJ/mol	Joback Method
ie	8.42	eV	NIST Webbook
ie	8.49 ± 0.05	eV	NIST Webbook
log10ws	-2.44		Crippen Method
logp	2.460		Crippen Method
mcvol	123.190	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	497.70	K	Joback Method
tc	723.71	K	Joback Method
tf	288.37	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.96	J/mol×K	497.70	Joback Method
cpg	246.81	J/mol×K	535.37	Joback Method
cpg	257.92	J/mol×K	573.04	Joback Method
cpg	268.33	J/mol×K	610.70	Joback Method
cpg	278.05	J/mol×K	648.37	Joback Method
cpg	287.12	J/mol×K	686.04	Joback Method
cpg	295.56	J/mol×K	723.71	Joback Method
dvisc	0.0022365	Pa×s	288.37	Joback Method
dvisc	0.0012738	Pa×s	323.26	Joback Method
dvisc	0.0008096	Pa×s	358.15	Joback Method
dvisc	0.0005577	Pa×s	393.04	Joback Method
dvisc	0.0004082	Pa×s	427.92	Joback Method
dvisc	0.0003132	Pa×s	462.81	Joback Method
dvisc	0.0002494	Pa×s	497.70	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.20	K	5.30	NIST Webbook

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=C589106&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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume