Benzene, (4-bromobutoxy)-

Other names:	(4-Bromobutoxy)benzene
	4-Bromobutyl phenyl ether
	1-Bromo-4-phenoxybutane
	Ether, 4-bromobutyl phenyl
	Phenoxybutyl bromide
	4-Phenoxybutyl bromide
Inchi:	InChI=1S/C10H13BrO/c11-8-4-5-9-12-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9H2
InchiKey:	QBLISOIWPZSVIK-UHFFFAOYSA-N
Formula:	C10H13BrO
SMILES:	BrCCCCOc1ccccc1
Mol. weight [g/mol]:	229.11
CAS:	1200-03-9

Physical Properties

Property code	Value	Unit	Source
gf	55.05	kJ/mol	Joback Method
hf	-119.09	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	48.97	kJ/mol	Joback Method
ie	8.54 ± 0.05	eV	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.240		Crippen Method
mcvol	151.370	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	543.46	K	Joback Method
tc	761.74	K	Joback Method
tf	310.91	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.38	J/mol×K	543.46	Joback Method
cpg	383.76	J/mol×K	725.36	Joback Method

cpg	373.03	J/mol×K	688.98	Joback Method
cpg	361.56	J/mol×K	652.60	Joback Method
cpg	349.31	J/mol×K	616.22	Joback Method
cpg	336.27	J/mol×K	579.84	Joback Method
cpg	393.79	J/mol×K	761.74	Joback Method
dvisc	0.0002093	Pa×s	543.46	Joback Method
dvisc	0.0002658	Pa×s	504.70	Joback Method
dvisc	0.0003514	Pa×s	465.94	Joback Method
dvisc	0.0004885	Pa×s	427.19	Joback Method
dvisc	0.0007253	Pa×s	388.43	Joback Method
dvisc	0.0011756	Pa×s	349.67	Joback Method
dvisc	0.0021493	Pa×s	310.91	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.70	K	2.40	NIST Webbook

Sources

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=C1200039&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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