Benzene, (3-bromopropoxy)-

Other names:	3-Phenoxypropyl bromide
	«gamma»-Phenoxypropyl bromide
	(3-Bromopropoxy)benzene
	Ether, 3-bromopropyl phenyl
	1-Bromo-3-phenoxypropane
	3-Bromopropyl phenyl ether
Inchi:	InChI=1S/C9H11BrO/c10-7-4-8-11-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2
InchiKey:	NIDWUZTTXGJFNN-UHFFFAOYSA-N
Formula:	C9H11BrO
SMILES:	BrCCCOc1ccccc1
Mol. weight [g/mol]:	215.09
CAS:	588-63-6

Physical Properties

Property code	Value	Unit	Source
gf	46.63	kJ/mol	Joback Method
hf	-98.45	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	46.75	kJ/mol	Joback Method
ie	8.56 ± 0.05	eV	NIST Webbook
log10ws	-2.86		Crippen Method
logp	2.850		Crippen Method
mcvol	137.280	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	520.58	K	Joback Method
tc	742.69	K	Joback Method
tf	299.64	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.73	J/mol×K	520.58	Joback Method
cpg	290.67	J/mol×K	557.60	Joback Method

cpg	302.82	J/mol×K	594.62	Joback Method
cpg	314.21	J/mol×K	631.64	Joback Method
cpg	324.86	J/mol×K	668.66	Joback Method
cpg	334.82	J/mol×K	705.68	Joback Method
cpg	344.11	J/mol×K	742.69	Joback Method
dvisc	0.0022066	Pa×s	299.64	Joback Method
dvisc	0.0012309	Pa×s	336.46	Joback Method
dvisc	0.0007704	Pa×s	373.29	Joback Method
dvisc	0.0005245	Pa×s	410.11	Joback Method
dvisc	0.0003805	Pa×s	446.93	Joback Method
dvisc	0.0002898	Pa×s	483.76	Joback Method
dvisc	0.0002294	Pa×s	520.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	1.90	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=C588636&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