Benzene, 1-bromo-4-phenoxy-

Other names:	Ether, p-bromophenyl phenyl p-(Phenoxy)bromobenzene p-Bromodiphenyl ether p-Bromophenoxybenzene p-Bromophenyl phenyl ether Diphenyl ether, 4-bromo- Ether, 4-bromophenyl phenyl Phenyl ether, 4-bromo- 1-Bromo-4-phenoxybenzene 4-Bromodiphenyl ether 4-Bromophenoxybenzene 4-Bromophenyl phenyl ether p-Bromphenyl phenyl ether p-Phenoxyphenyl bromide 4-Phenoxy-1-bromobenzene NSC 5619
Inchi:	InChI=1S/C12H9BrO/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9H
InchiKey:	JDUYPUMQALQRCN-UHFFFAOYSA-N
Formula:	C12H9BrO
SMILES:	Brc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	249.10
CAS:	101-55-3

Physical Properties

Property code	Value	Unit	Source
gf	174.67	kJ/mol	Joback Method
hf	64.69	kJ/mol	Joback Method
hfus	21.00	kJ/mol	Joback Method
hvap	56.36	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.241		Crippen Method
mcvol	155.790	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	285.80		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1661.70		NIST Webbook

rinpol	1641.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	285.80		NIST Webbook
ripol	2394.00		NIST Webbook
ripol	2394.00		NIST Webbook
tb	578.20	K	NIST Webbook
tc	881.79	K	Joback Method
tf	291.90 ± 0.02	K	NIST Webbook
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.34	J/mol×K	881.79	Joback Method
cpg	397.66	J/mol×K	838.31	Joback Method
cpg	388.07	J/mol×K	794.82	Joback Method
cpg	377.50	J/mol×K	751.34	Joback Method
cpg	365.88	J/mol×K	707.85	Joback Method
cpg	353.16	J/mol×K	664.37	Joback Method
cpg	339.25	J/mol×K	620.88	Joback Method
dvisc	0.0012460	Pa×s	372.39	Joback Method
dvisc	0.0001683	Pa×s	620.88	Joback Method
dvisc	0.0002085	Pa×s	579.46	Joback Method
dvisc	0.0002671	Pa×s	538.05	Joback Method
dvisc	0.0003565	Pa×s	496.63	Joback Method
dvisc	0.0005014	Pa×s	455.22	Joback Method
dvisc	0.0007553	Pa×s	413.81	Joback Method
hvapt	64.60	kJ/mol	568.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.00 ± 2.00	K	0.45	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=C101553&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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	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