4-Bromophenyl ether

Other names:	di(4-Bromophenyl)ether
	4,4'-Dibromodiphenyl ether
	Bis(p-bromophenyl)ether
	Bis-(4-bromophenyl) ether
	Benzene, 1,1'-oxybis[4-bromo-
	p,p'-Dibromodiphenyl ether
	Bis(bromophenyl) ether
	Ether, bis(p-bromophenyl)
	Ether, bis(4-bromophenyl)
	USAF DO-61
	Diphenyl ether, 4,4'-dibromo
	NSC 1787
	NSC 9487
	4,4'-BDE
Inchi:	InChI=1S/C12H8Br2O/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H
InchiKey:	YAWIAFUBXXPJMQ-UHFFFAOYSA-N
Formula:	C12H8Br2O
SMILES:	Brc1ccc(Oc2ccc(Br)cc2)cc1
Mol. weight [g/mol]:	328.00
CAS:	2050-47-7

Physical Properties

Property code	Value	Unit	Source
gf	179.36	kJ/mol	Joback Method
hf	79.55	kJ/mol	Joback Method
hfus	25.90	kJ/mol	Joback Method
hvap	63.46	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.004		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
rinpol	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook
tb	612.20	K	NIST Webbook
tc	965.48	K	Joback Method
tf	327.15 ± 1.50	K	NIST Webbook
tf	327.15 ± 1.50	K	NIST Webbook

vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.09	J/mol×K	692.02	Joback Method
cpg	382.04	J/mol×K	737.60	Joback Method
cpg	392.89	J/mol×K	783.17	Joback Method
cpg	402.71	J/mol×K	828.75	Joback Method
cpg	411.60	J/mol×K	874.33	Joback Method
cpg	419.63	J/mol×K	919.91	Joback Method
cpg	426.89	J/mol×K	965.48	Joback Method
dvisc	0.0008047	Pa×s	444.71	Joback Method
dvisc	0.0005395	Pa×s	485.93	Joback Method
dvisc	0.0003850	Pa×s	527.15	Joback Method
dvisc	0.0002886	Pa×s	568.37	Joback Method
dvisc	0.0002249	Pa×s	609.58	Joback Method
dvisc	0.0001809	Pa×s	650.80	Joback Method
dvisc	0.0001493	Pa×s	692.02	Joback Method
hvapt	78.00	kJ/mol	418.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050477&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume