1,3-Benzenediol, 4-bromo-

Other names:	1-Bromo-2,4-dihydroxybenzene
	4-Bromo-1,3-dihydroxybenzene
	4-Bromoresorcinol
	Resorcinol, 4-bromo-
Inchi:	InChI=1S/C6H5BrO2/c7-5-2-1-4(8)3-6(5)9/h1-3,8-9H
InchiKey:	MPCCNXGZCOXPMG-UHFFFAOYSA-N
Formula:	C6H5BrO2
SMILES:	Oc1ccc(Br)c(O)c1
Mol. weight [g/mol]:	189.01
CAS:	6626-15-9

Physical Properties

Property code	Value	Unit	Source
gf	-182.87	kJ/mol	Joback Method
hf	-258.93	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.860		Crippen Method
mcvol	100.880	ml/mol	McGowan Method
pc	8324.90	kPa	Joback Method
tb	590.76	K	Joback Method
tc	854.07	K	Joback Method
tf	467.04	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.71	J/mol×K	590.76	Joback Method
cpg	217.40	J/mol×K	634.64	Joback Method
cpg	223.38	J/mol×K	678.53	Joback Method
cpg	228.85	J/mol×K	722.41	Joback Method
cpg	234.01	J/mol×K	766.30	Joback Method

cpg	239.05	J/mol×K	810.18	Joback Method
cpg	244.17	J/mol×K	854.07	Joback Method
dvisc	0.0001699	Pa×s	467.04	Joback Method
dvisc	0.0000968	Pa×s	487.66	Joback Method
dvisc	0.0000577	Pa×s	508.28	Joback Method
dvisc	0.0000358	Pa×s	528.90	Joback Method
dvisc	0.0000230	Pa×s	549.52	Joback Method
dvisc	0.0000153	Pa×s	570.14	Joback Method
dvisc	0.0000105	Pa×s	590.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.20	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6626159&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
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