Benzaldehyde, 4-bromo-

Other names:	4-Brombenzaldehyd
	4-bromobenzaldehyde
	Benzaldehyde, p-bromo-
	p-bromobenzaldehyde
Inchi:	InChI=1S/C7H5BrO/c8-7-3-1-6(5-9)2-4-7/h1-5H
InchiKey:	ZRYZBQLXDKPBDU-UHFFFAOYSA-N
Formula:	C7H5BrO
SMILES:	O=Cc1ccc(Br)cc1
Mol. weight [g/mol]:	185.02
CAS:	1122-91-4

Physical Properties

Property code	Value	Unit	Source
gf	25.64	kJ/mol	Joback Method
hf	-22.00	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Phase Equilibria of Acrylonitrile and p-Bromobenzaldehyde in Carbon Dioxide
hvap	47.27	kJ/mol	Joback Method
ie	9.22	eV	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.262		Crippen Method
mcvol	104.800	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
rinpol	1207.10		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1216.50		NIST Webbook
tb	506.04	K	Joback Method
tc	744.20	K	Joback Method
tf	329.15 ± 2.00	K	NIST Webbook
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.30	J/mol×K	744.20	Joback Method
cpg	186.18	J/mol×K	506.04	Joback Method
cpg	195.09	J/mol×K	545.73	Joback Method
cpg	203.32	J/mol×K	585.43	Joback Method
cpg	210.92	J/mol×K	625.12	Joback Method
cpg	217.93	J/mol×K	664.81	Joback Method
cpg	224.37	J/mol×K	704.51	Joback Method
dvisc	0.0003736	Pa×s	506.04	Joback Method
dvisc	0.0022488	Pa×s	309.39	Joback Method
dvisc	0.0014448	Pa×s	342.16	Joback Method
dvisc	0.0010028	Pa×s	374.94	Joback Method
dvisc	0.0007382	Pa×s	407.71	Joback Method
dvisc	0.0005687	Pa×s	440.49	Joback Method
dvisc	0.0004543	Pa×s	473.26	Joback Method
hfust	22.60	kJ/mol	334.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase Equilibria of Acrylonitrile and p-Bromobenzaldehyde in Carbon Dioxide:	https://www.doi.org/10.1021/je700448v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume