Benzaldehyde, 2-bromo-

Other names: Benzaldehyde, o-bromo-
o-Bromobenzaldehyde
2-Bromobenzaldehyde
Inchi: InChI=1S/C7H5BrO/c8-7-4-2-1-3-6(7)5-9/h1-5H
InchiKey: NDOPHXWIAZIXPR-UHFFFAOYSA-N
Formula: C7H5BrO
SMILES: O=Cc1ccccc1Br
Mol. weight [g/mol]: 185.02
CAS: 6630-33-7

Physical Properties

Property code	Value	Unit	Source
gf	25.64	kJ/mol	Joback Method
hf	-22.00	kJ/mol	Joback Method
hfus	15.11	kJ/mol	Joback Method
hvap	47.27	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.262		Crippen Method
mcvol	104.800	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
rinpol	1204.70		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1211.60		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1838.00		NIST Webbook
tb	503.20	K	NIST Webbook
tb	503.00	K	NIST Webbook
tc	744.20	K	Joback Method
tf	295.00	K	NIST Webbook
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	186.18	J/mol×K	506.04	Joback Method
cpg	224.37	J/mol×K	704.51	Joback Method
cpg	217.93	J/mol×K	664.81	Joback Method
cpg	210.92	J/mol×K	625.12	Joback Method
cpg	203.32	J/mol×K	585.43	Joback Method
cpg	195.09	J/mol×K	545.73	Joback Method
cpg	230.30	J/mol×K	744.20	Joback Method
dvisc	0.0003736	Pa×s	506.04	Joback Method
dvisc	0.0004543	Pa×s	473.26	Joback Method
dvisc	0.0005687	Pa×s	440.49	Joback Method
dvisc	0.0007382	Pa×s	407.71	Joback Method
dvisc	0.0010028	Pa×s	374.94	Joback Method
dvisc	0.0014448	Pa×s	342.16	Joback Method
dvisc	0.0022488	Pa×s	309.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.20	K	1.60	NIST Webbook
tbrp	391.50 ± 0.50	K	1.60	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6630337&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
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

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
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