Benzaldehyde, 4-butoxy-

Other names:	4-Butoxybenzaldehyde
	p-Butoxybenzaldehyde
	p-(n-Butoxy)benzaldehyde
	Benzaldehyde, p-butoxy-
Inchi:	InChI=1S/C11H14O2/c1-2-3-8-13-11-6-4-10(9-12)5-7-11/h4-7,9H,2-3,8H2,1H3
InchiKey:	XHWMNHADTZZHGI-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCCCOc1ccc(C=O)cc1
Mol. weight [g/mol]:	178.23
CAS:	5736-88-9

Physical Properties

Property code	Value	Unit	Source
gf	-60.00	kJ/mol	Joback Method
hf	-263.11	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.678		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
tb	558.20	K	NIST Webbook
tc	759.25	K	Joback Method
tf	316.90	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.98	J/mol×K	553.82	Joback Method
cpg	360.79	J/mol×K	588.06	Joback Method
cpg	373.87	J/mol×K	622.30	Joback Method
cpg	386.25	J/mol×K	656.54	Joback Method
cpg	397.93	J/mol×K	690.78	Joback Method

cpg	408.93	J/mol×K	725.01	Joback Method
cpg	419.27	J/mol×K	759.25	Joback Method
dvisc	0.0019634	Pa×s	316.90	Joback Method
dvisc	0.0011054	Pa×s	356.39	Joback Method
dvisc	0.0006979	Pa×s	395.87	Joback Method
dvisc	0.0004790	Pa×s	435.36	Joback Method
dvisc	0.0003500	Pa×s	474.85	Joback Method
dvisc	0.0002683	Pa×s	514.33	Joback Method
dvisc	0.0002137	Pa×s	553.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.00 ± 1.00	K	2.40	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5736889&Units=SI

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