

4-Butoxybenzyl alcohol

Other names:	p-Butoxybenzyl alcohol Benzenemethanol, 4-butoxy-
Inchi:	InChI=1S/C11H16O2/c1-2-3-8-13-11-6-4-10(9-12)5-7-11/h4-7,12H,2-3,8-9H2,1H3
InchiKey:	MGKNBDBZIKPUFM-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	CCCCOc1ccc(CO)cc1
Mol. weight [g/mol]:	180.24
CAS:	6214-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-97.30	kJ/mol	Joback Method
hf	-329.76	kJ/mol	Joback Method
hfus	23.17	kJ/mol	Joback Method
hvap	62.11	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.358		Crippen Method
mvol	153.830	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
tb	597.34	K	Joback Method
tc	787.04	K	Joback Method
tf	335.72	K	Joback Method
vc	0.581	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.03	J/molxK	597.34	Joback Method
cpg	395.82	J/molxK	628.96	Joback Method
cpg	407.97	J/molxK	660.57	Joback Method
cpg	419.50	J/molxK	692.19	Joback Method
cpg	430.43	J/molxK	723.81	Joback Method
cpg	440.78	J/molxK	755.43	Joback Method
cpg	450.54	J/molxK	787.04	Joback Method

dvisc	0.0040576	Paxs	335.72	Joback Method
dvisc	0.0013705	Paxs	379.32	Joback Method
dvisc	0.0005790	Paxs	422.93	Joback Method
dvisc	0.0002874	Paxs	466.53	Joback Method
dvisc	0.0001608	Paxs	510.13	Joback Method
dvisc	0.0000986	Paxs	553.74	Joback Method
dvisc	0.0000649	Paxs	597.34	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.00 ± 1.00	K	1.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6214455&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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

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