

P-BUTOXYBENZYL ALCOHOL

Other names:	Benzenemethanol, 4-butoxy- p-Butoxybenzyl alcohol
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]:	180.25

Physical Properties

Property code	Value	Unit	Source
hfus	23.17	kJ/mol	Joback Method
ie	8.16	eV	Cheméo Relay (1.0)
log10ws	-2.57		Cheméo Relay (1.0)
logp	2.358		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
tb	547.44	K	Cheméo Relay (1.0)
tc	755.35	K	Cheméo Relay (1.0)
tf	304.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.03	J/mol×K	597.34	Joback Method
cpg	395.82	J/mol×K	628.96	Joback Method
cpg	407.97	J/mol×K	660.57	Joback Method
cpg	419.50	J/mol×K	692.19	Joback Method
cpg	430.43	J/mol×K	723.81	Joback Method
cpg	440.78	J/mol×K	755.43	Joback Method
cpg	450.54	J/mol×K	787.04	Joback Method
dvisc	0.0040576	Pa×s	335.72	Joback Method
dvisc	0.0013705	Pa×s	379.32	Joback Method
dvisc	0.0005790	Pa×s	422.93	Joback Method
dvisc	0.0002874	Pa×s	466.53	Joback Method
dvisc	0.0001608	Pa×s	510.13	Joback Method

dvisc	0.0000986	Pa×s	553.74	Joback Method
dvisc	0.0000649	Pa×s	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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6214455&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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