p-Bromobenzylalcohol

Other names: Benzyl alcohol, p-bromo-
p-Bromobenzyl alcohol
4-Bromobenzyl alcohol
Inchi: InChI=1S/C7H7BrO/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2
InchiKey: VEDDBHYQWFOITD-UHFFFAOYSA-N
Formula: C7H7BrO
SMILES: OCc1ccc(Br)cc1
Mol. weight [g/mol]: 187.04

Physical Properties

Property code	Value	Unit	Source
hf	-90.77	kJ/mol	Cheméo Relay (1.0)
hfus	16.91	kJ/mol	Joback Method
hvap	81.20	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-1.87		Cheméo Relay (1.0)
logp	1.941		Crippen Method
mcvol	109.100	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	516.45	K	Cheméo Relay (1.0)
tc	775.93	K	Cheméo Relay (1.0)
tf	327.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.18	J/mol×K	549.56	Joback Method
cpg	221.65	J/mol×K	585.59	Joback Method
cpg	229.56	J/mol×K	621.61	Joback Method
cpg	236.93	J/mol×K	657.64	Joback Method
cpg	243.80	J/mol×K	693.66	Joback Method
cpg	250.21	J/mol×K	729.69	Joback Method
cpg	256.18	J/mol×K	765.72	Joback Method
dvisc	0.0052897	Pa×s	328.21	Joback Method

dvisc	0.0021291	Pa×s	365.10	Joback Method
dvisc	0.0010127	Pa×s	401.99	Joback Method
dvisc	0.0005458	Pa×s	438.88	Joback Method
dvisc	0.0003238	Pa×s	475.78	Joback Method
dvisc	0.0002070	Pa×s	512.67	Joback Method
dvisc	0.0001406	Pa×s	549.56	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C873756&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

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point