3-Bromobenzyl alcohol

Other names: m-Bromobenzyl alcohol
Benzenemethanol, 3-bromo-
Inchi: InChI=1S/C7H7BrO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5H2
InchiKey: FSWNRRSWFBXQCL-UHFFFAOYSA-N
Formula: C7H7BrO
SMILES: OCc1cccc(Br)c1
Mol. weight [g/mol]: 187.03
CAS: 15852-73-0

Physical Properties

Property code	Value	Unit	Source
gf	-11.66	kJ/mol	Joback Method
hf	-88.65	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.941		Crippen Method
mcvol	109.100	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	549.56	K	Joback Method
tc	765.72	K	Joback Method
tf	328.21	K	Joback Method
vc	0.401	m3/kmol	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.20	K	2.10	NIST Webbook
tbrp	438.00	K	2.10	NIST Webbook
tbrp	525.50 ± 0.50	K	94.80	NIST Webbook
tbrp	514.00 ± 16.00	K	98.40	NIST Webbook
tbrp	364.30 ± 0.70	K	0.09	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=C15852730&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