Benzeneethanol, 4-bromo-

Other names:	Phenethyl alcohol, p-bromo-
	4-Bromo-phenethyl alcohol
	2-(4-Bromophenyl)ethanol
	p-Bromophenethyl alcohol
Inchi:	InChI=1S/C8H9BrO/c9-8-3-1-7(2-4-8)5-6-10/h1-4,10H,5-6H2
InchiKey:	PMOSJSPFNDUAFY-UHFFFAOYSA-N
Formula:	C8H9BrO
SMILES:	OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	201.06
CAS:	4654-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-3.24	kJ/mol	Joback Method
hf	-109.29	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	1.984		Crippen Method
mcvol	123.190	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
ripol	2546.00		NIST Webbook
ripol	2546.00		NIST Webbook
tb	572.44	K	Joback Method
tc	784.97	K	Joback Method
tf	339.48	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.51	J/mol×K	572.44	Joback Method
cpg	266.02	J/mol×K	607.86	Joback Method
cpg	274.92	J/mol×K	643.28	Joback Method

cpg	283.24	J/mol×K	678.71	Joback Method
cpg	291.02	J/mol×K	714.13	Joback Method
cpg	298.30	J/mol×K	749.55	Joback Method
cpg	305.10	J/mol×K	784.97	Joback Method
dvisc	0.0045605	Pa×s	339.48	Joback Method
dvisc	0.0018135	Pa×s	378.31	Joback Method
dvisc	0.0008562	Pa×s	417.13	Joback Method
dvisc	0.0004594	Pa×s	455.96	Joback Method
dvisc	0.0002718	Pa×s	494.79	Joback Method
dvisc	0.0001735	Pa×s	533.61	Joback Method
dvisc	0.0001178	Pa×s	572.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.20	K	1.00	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=C4654391&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume