p-Bromobenzylamine

Other names:	Benzenemethanamine, 4-bromo- 4-Bromobenzylamine
Inchi:	InChI=1S/C7H8BrN/c8-7-3-1-6(5-9)2-4-7/h1-4H,5,9H2
InchiKey:	XRNVSPDQTPVECU-UHFFFAOYSA-N
Formula:	C7H8BrN
SMILES:	NCc1ccc(Br)cc1
Mol. weight [g/mol]:	186.05
CAS:	3959-07-7

Physical Properties

Property code	Value	Unit	Source
gf	191.61	kJ/mol	Joback Method
hf	97.37	kJ/mol	Joback Method
hfus	18.02	kJ/mol	Joback Method
hvap	51.19	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	1.908		Crippen Method
mcvol	113.210	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	523.00	K	NIST Webbook
tc	774.87	K	Joback Method
tf	293.00	K	NIST Webbook
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.82	J/mol×K	529.91	Joback Method
cpg	231.34	J/mol×K	570.74	Joback Method
cpg	241.08	J/mol×K	611.56	Joback Method
cpg	250.09	J/mol×K	652.39	Joback Method
cpg	258.42	J/mol×K	693.21	Joback Method
cpg	266.10	J/mol×K	734.04	Joback Method
cpg	273.20	J/mol×K	774.87	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.50 ± 0.50	K	2.00	NIST Webbook

Sources

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=C3959077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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

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