N-methyl-o-bromobenzylamine

Inchi: InChI=1S/C8H10BrN/c1-10-6-7-4-2-3-5-8(7)9/h2-5,10H,6H2,1H3
InchiKey: TUADRPBKJHMHDH-UHFFFAOYSA-N
Formula: C8H10BrN
SMILES: CNCc1ccccc1Br
Mol. weight [g/mol]: 200.08
CAS: 698-19-1

Physical Properties

Property code	Value	Unit	Source
gf	222.97	kJ/mol	Joback Method
hf	96.41	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	49.21	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.168		Crippen Method
mcvol	127.300	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	530.43	K	Joback Method
tc	760.39	K	Joback Method
tf	331.32	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.27	J/mol×K	530.43	Joback Method
cpg	267.23	J/mol×K	568.76	Joback Method
cpg	278.39	J/mol×K	607.08	Joback Method
cpg	288.79	J/mol×K	645.41	Joback Method
cpg	298.46	J/mol×K	683.74	Joback Method
cpg	307.45	J/mol×K	722.07	Joback Method
cpg	315.82	J/mol×K	760.39	Joback Method

Sources

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=C698191&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume