(+)-p-Bromo-«alpha»-phenethylamine

Other names: Benzenemethanamine, 4-bromo-«alpha»-methyl-, (R)-
(R)-4-bromo-«alpha»-methylbenzylamine
Inchi: InChI=1S/C8H10BrN/c1-6(10)7-2-4-8(9)5-3-7/h2-6H,10H2,1H3
InchiKey: SOZMSEPDYJGBEK-UHFFFAOYSA-N
Formula: C8H10BrN
SMILES: CC(N)c1ccc(Br)cc1
Mol. weight [g/mol]: 200.08
CAS: 45791-36-4

Physical Properties

Property code	Value	Unit	Source
gf	197.59	kJ/mol	Joback Method
hf	71.45	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	53.03	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.469		Crippen Method
mcvol	127.300	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	552.35	K	Joback Method
tc	797.97	K	Joback Method
tf	346.92	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.20	J/mol×K	552.35	Joback Method
cpg	276.20	J/mol×K	593.29	Joback Method
cpg	287.32	J/mol×K	634.22	Joback Method
cpg	297.61	J/mol×K	675.16	Joback Method
cpg	307.13	J/mol×K	716.09	Joback Method
cpg	315.91	J/mol×K	757.03	Joback Method
cpg	324.03	J/mol×K	797.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C45791364&Units=SI
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

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