

(-)-1-(4-Bromophenyl)ethylamine

Other names:	Benzenemethanamine, 4-bromo-«alpha»-methyl-, («alpha»S)-(S)-(-)-1-(4-BROMOPHENYL)ETHYLAMINE
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:	27298-97-1

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C27298971&Units=SI

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

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