Dl-p-hydroxy-alpha-methylphenethyl amine hydrobromide

Inchi: InChI=1S/C9H13NO/c1-7(6-10)8-2-4-9(11)5-3-8/h2-5,7,11H,6,10H2,1H3

InchiKey: ZGYDQXZKRDEGFR-UHFFFAOYSA-N

Formula: C9H13NO

SMILES: CC(CN)c1ccc(O)cc1

Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
gf	46.70	kJ/mol	Joback Method
hf	-141.36	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	61.17	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.454		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	584.71	K	Joback Method
tc	820.97	K	Joback Method
tf	397.59	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.24	J/mol×K	584.71	Joback Method
cpg	335.07	J/mol×K	624.09	Joback Method
cpg	346.96	J/mol×K	663.46	Joback Method
cpg	358.00	J/mol×K	702.84	Joback Method
cpg	368.30	J/mol×K	742.22	Joback Method
cpg	377.94	J/mol×K	781.59	Joback Method
cpg	387.03	J/mol×K	820.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003615&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