5-Amino-2-methoxyphenol

Other names: 3-Hydroxy-4-methoxyaniline
Phenol, 5-amino-2-methoxy-
Inchi: InChI=1S/C7H9NO2/c1-10-7-3-2-5(8)4-6(7)9/h2-4,9H,8H2,1H3
InchiKey: BLQFHJKRTDIZLX-UHFFFAOYSA-N
Formula: C7H9NO2
SMILES: COc1ccc(N)cc1O
Mol. weight [g/mol]: 139.15
CAS: 1687-53-2

Physical Properties

Property code	Value	Unit	Source
gf	-82.33	kJ/mol	Joback Method
hf	-238.49	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	60.18	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.983		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
tb	566.79	K	Joback Method
tc	805.05	K	Joback Method
tf	424.80	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.20	J/mol×K	566.79	Joback Method
cpg	263.24	J/mol×K	606.50	Joback Method
cpg	272.60	J/mol×K	646.21	Joback Method
cpg	281.34	J/mol×K	685.92	Joback Method
cpg	289.52	J/mol×K	725.63	Joback Method
cpg	297.21	J/mol×K	765.34	Joback Method
cpg	304.46	J/mol×K	805.05	Joback Method

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=C1687532&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume