Methyl 3-amino-4-hydroxybenzoate

Other names:	Benzoic acid, 3-amino-4-hydroxy-, methyl ester
	Aminobenz
	Methyl m-amino-p-hydroxybenzoate
	Methyl 4-hydroxy-3-aminobenzoate
	Orthocaine
	Orthoderm
	Orthoform
	3-Amino-4-hydroxybenzoic acid methyl ester
	Orthoform new
	NSC 9813
Inchi:	InChI=1S/C8H9NO3/c1-12-8(11)5-2-3-7(10)6(9)4-5/h2-4,10H,9H2,1H3
InchiKey:	VNQABZCSYCTZMS-UHFFFAOYSA-N
Formula:	C8H9NO3
SMILES:	COC(=O)c1ccc(O)c(N)c1
Mol. weight [g/mol]:	167.16
CAS:	536-25-4

Physical Properties

Property code	Value	Unit	Source
gf	-202.83	kJ/mol	Joback Method
hf	-371.71	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	69.15	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.761		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4973.33	kPa	Joback Method
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
tb	643.54	K	Joback Method
tc	883.84	K	Joback Method
tf	486.00	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.53	J/mol×K	643.54	Joback Method
cpg	317.32	J/mol×K	683.59	Joback Method
cpg	326.45	J/mol×K	723.64	Joback Method
cpg	334.97	J/mol×K	763.69	Joback Method
cpg	342.95	J/mol×K	803.74	Joback Method
cpg	350.46	J/mol×K	843.79	Joback Method
cpg	357.56	J/mol×K	883.84	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=C536254&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume