Benzenamine, 3,4-dimethoxy-

Other names:	Aniline, 3,4-dimethoxy-
	2-Methoxy-4-aminoanisole
	3,4-Dimethoxyaniline
	4-Aminoveratrol
	4-Aminoveratrole
Inchi:	InChI=1S/C8H11NO2/c1-10-7-4-3-6(9)5-8(7)11-2/h3-5H,9H2,1-2H3
InchiKey:	LGDHZCLREKIGKJ-UHFFFAOYSA-N
Formula:	C8H11NO2
SMILES:	COc1ccc(N)cc1OC
Mol. weight [g/mol]:	153.18
CAS:	6315-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-33.92	kJ/mol	Joback Method
hf	-225.51	kJ/mol	Joback Method
hfus	17.31	kJ/mol	Joback Method
hvap	52.46	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.286		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
tb	536.45	K	Joback Method
tc	757.02	K	Joback Method
tf	359.10	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.40	J/mol×K	536.45	Joback Method
cpg	285.22	J/mol×K	573.21	Joback Method
cpg	296.50	J/mol×K	609.97	Joback Method
cpg	307.24	J/mol×K	646.74	Joback Method

cpg	317.42	J/mol×K	683.50	Joback Method
cpg	327.03	J/mol×K	720.26	Joback Method
cpg	336.07	J/mol×K	757.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.20	K	2.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6315895&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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