Benzenamine, 3,5-dimethoxy-

Other names: 3,5-Dimethoxybenzeneamine
3,5-Dimethoxyaniline
Inchi: InChI=1S/C8H11NO2/c1-10-7-3-6(9)4-8(5-7)11-2/h3-5H,9H2,1-2H3
InchiKey: WNRGWPVJGDABME-UHFFFAOYSA-N
Formula: C8H11NO2
SMILES: COc1cc(N)cc(OC)c1
Mol. weight [g/mol]: 153.18
CAS: 10272-07-8

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	451.20	K	2.70	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10272078&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume