Benzenamine, 4-chloro-2,5-dimethoxy-

Other names:	1-amino-4-chloro-2,5-dimethoxybenzene
	2,5-dimethoxy-4-chloroaniline
	4-chloro-2,5-dimethoxyaniline
	4-chloro-2,5-dimethoxybenzenamine
	Aniline, 4-chloro-2,5-dimethoxy-
Inchi:	InChI=1S/C8H10ClNO2/c1-11-7-4-6(10)8(12-2)3-5(7)9/h3-4H,10H2,1-2H3
InchiKey:	YGUFQYGSBVXPMC-UHFFFAOYSA-N
Formula:	C8H10ClNO2
SMILES:	COc1cc(Cl)c(OC)cc1N
Mol. weight [g/mol]:	187.62
CAS:	6358-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-55.48	kJ/mol	Joback Method
hf	-252.72	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	57.51	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.939		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	578.86	K	Joback Method
tc	804.78	K	Joback Method
tf	391.85	K	Measurement and correlation of solubility of 4-chloro-2,5-dimethoxynitrobenzene and 4-chloro-2,5-dimethoxyaniline in methanol, ethanol, xylene and toluene
tt	389.38	K	Solubility of 4-Chloro-2,5-dimethoxynitrobenzene, 4-Chloro-2,5-dimethoxyaniline, and 2,5-Dimethoxyaniline in Binary and Pure Solvents: Determination and Modeling
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.21	J/mol×K	578.86	Joback Method
cpg	307.15	J/mol×K	616.51	Joback Method
cpg	317.56	J/mol×K	654.17	Joback Method
cpg	327.43	J/mol×K	691.82	Joback Method
cpg	336.75	J/mol×K	729.48	Joback Method
cpg	345.48	J/mol×K	767.13	Joback Method
cpg	353.63	J/mol×K	804.78	Joback Method

Sources

Measurement and correlation of solubility of 4-Chloro-2,5-dimethoxynitrobenzene and 4-Chloro-2,5-dimethoxyaniline in methanol+ethanol, xylene and toluene:	https://www.doi.org/10.1016/j.jct.2014.09.003
Solubility of 4-Chloro-2,5-dimethoxynitrobenzene and 4-Chloro-2,5-dimethoxyaniline in Joback Method:	https://www.doi.org/10.1021/acs.jced.9b00011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of 4-Chloro-2,5-dimethoxyaniline and 2,5-Dimethoxyaniline in Binary and Pure Solvents: Determination and Modeling:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6358641&Units=SI
NIST Webbook:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen 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
tt:	Triple Point Temperature

vc: Critical Volume