Benzoic acid, 2-amino-5-chloro-, methyl ester

Other names:	Anthranilic acid, 5-chloro-, methyl ester
	Methyl 2-amino-5-chlorobenzoate
	Methyl 5-chloroanthranilate
Inchi:	InChI=1S/C8H8ClNO2/c1-12-8(11)6-4-5(9)2-3-7(6)10/h2-4H,10H2,1H3
InchiKey:	IGHVUURTQGBABT-UHFFFAOYSA-N
Formula:	C8H8ClNO2
SMILES:	COC(=O)c1cc(Cl)ccc1N
Mol. weight [g/mol]:	185.61
CAS:	5202-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-69.77	kJ/mol	Joback Method
hf	-221.61	kJ/mol	Joback Method
hfus	21.92	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.709		Crippen Method
mcvol	129.480	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	605.33	K	Joback Method
tc	840.85	K	Joback Method
tf	342.00 ± 1.00	K	NIST Webbook
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.11	J/mol×K	605.33	Joback Method
cpg	296.27	J/mol×K	644.58	Joback Method
cpg	305.78	J/mol×K	683.84	Joback Method
cpg	314.63	J/mol×K	723.09	Joback Method
cpg	322.85	J/mol×K	762.35	Joback Method
cpg	330.43	J/mol×K	801.60	Joback Method

cpg	337.38	J/mol×K	840.85	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	442.20	K	2.90	NIST Webbook
tbrp	424.50 ± 1.50	K	1.30	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=C5202891&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