

2-Amino-5-chlorobenzamide

Other names:	Benzamide, 2-amino-5-chloro-5-Chloroanthranilamide
Inchi:	InChI=1S/C7H7ClN2O/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H2,10,11)
InchiKey:	DNRVZOZGQHHDAT-UHFFFAOYSA-N
Formula:	C7H7ClN2O
SMILES:	NC(=O)c1cc(Cl)ccc1N
Mol. weight [g/mol]:	170.60
CAS:	5202-85-7

Physical Properties

Property code	Value	Unit	Source
gf	93.26	kJ/mol	Joback Method
hf	-34.96	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.021		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	632.56	K	Joback Method
tc	883.78	K	Joback Method
tf	466.48	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.79	J/mol×K	632.56	Joback Method
cpg	276.79	J/mol×K	674.43	Joback Method
cpg	285.09	J/mol×K	716.30	Joback Method
cpg	292.72	J/mol×K	758.17	Joback Method
cpg	299.70	J/mol×K	800.04	Joback Method
cpg	306.06	J/mol×K	841.91	Joback Method
cpg	311.84	J/mol×K	883.78	Joback Method

Sources

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=C5202857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
vc:	Critical Volume

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