3-Chlorobenzamide

Other names: m-Chlorobenzamide
Benzamide, 3-chloro-
Inchi: InChI=1S/C7H6ClNO/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H2,9,10)
InchiKey: MJTGQALMWUUPQM-UHFFFAOYSA-N
Formula: C7H6ClNO
SMILES: NC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 155.58
CAS: 618-48-4

Physical Properties

Property code	Value	Unit	Source
affp	877.20	kJ/mol	NIST Webbook
basg	846.30	kJ/mol	NIST Webbook
gf	36.44	kJ/mol	Joback Method
hf	-57.28	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
ie	9.34	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	1.439		Crippen Method
mcvol	109.520	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	555.05	K	Joback Method
tc	798.07	K	Joback Method
tf	370.70	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.12	J/mol×K	555.05	Joback Method
cpg	231.55	J/mol×K	595.55	Joback Method
cpg	240.26	J/mol×K	636.06	Joback Method
cpg	248.30	J/mol×K	676.56	Joback Method

cpg	255.70	J/mol×K	717.06	Joback Method
cpg	262.48	J/mol×K	757.56	Joback Method
cpg	268.69	J/mol×K	798.07	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=C618484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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