2-Amino-6-chlorobenzonitrile

Other names: 2-Amino-6-chlorobenzonitrile
6-Amino-2-chlorobenzonitrile
Benzonitrile, 2-amino-6-chloro-
Inchi: InChI=1S/C7H5ClN2/c8-6-2-1-3-7(10)5(6)4-9/h1-3H,10H2
InchiKey: MEJVTQKBWPYBFG-UHFFFAOYSA-N
Formula: C7H5ClN2
SMILES: N#Cc1c(N)cccc1Cl
Mol. weight [g/mol]: 152.58

Physical Properties

Property code	Value	Unit	Source
hfus	18.05	kJ/mol	Joback Method
hvap	69.01	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
log10ws	-2.30		Cheméo Relay (1.0)
logp	1.794		Crippen Method
mcvol	109.330	ml/mol	McGowan Method
tb	567.67	K	Cheméo Relay (1.0)
tf	396.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.84	J/mol×K	608.24	Joback Method
cpg	231.65	J/mol×K	650.15	Joback Method
cpg	238.88	J/mol×K	692.06	Joback Method
cpg	245.54	J/mol×K	733.97	Joback Method
cpg	251.68	J/mol×K	775.87	Joback Method
cpg	257.31	J/mol×K	817.78	Joback Method
cpg	262.46	J/mol×K	859.69	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6575117&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point