

Phenol, 2-amino-6-chloro-

Inchi:	InChI=1S/C6H6ClNO/c7-4-2-1-3-5(8)6(4)9/h1-3,9H,8H2
InchiKey:	QUUIUKFPLUUSGQ-UHFFFAOYSA-N
Formula:	C6H6ClNO
SMILES:	Nc1cccc(Cl)c1O
Mol. weight [g/mol]:	143.57

Physical Properties

Property code	Value	Unit	Source
gf	2.32	kJ/mol	Joback Method
hf	-101.37	kJ/mol	Joback Method
hfus	20.13	kJ/mol	Joback Method
hvap	59.93	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.628		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
pc	5836.07	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
tb	558.92	K	Joback Method
tc	810.11	K	Joback Method
tf	421.22	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.45	J/mol×K	558.92	Joback Method
cpg	218.57	J/mol×K	600.79	Joback Method
cpg	225.98	J/mol×K	642.65	Joback Method
cpg	232.78	J/mol×K	684.52	Joback Method
cpg	239.06	J/mol×K	726.38	Joback Method
cpg	244.92	J/mol×K	768.25	Joback Method
cpg	250.45	J/mol×K	810.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U362588&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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