2,3,4,5,6-Pentachloroaniline

Other names:	Benzenamine, 2,3,4,5,6-pentachloro- Aniline, 2,3,4,5,6-pentachloro- Pentachloroaminobenzene Pentachloroaniline PCA 2,3,4,5,6-Pentachlorobenzenamine
Inchi:	InChI=1S/C6H2Cl5N/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H2
InchiKey:	KHCZSJXTDDHLGJ-UHFFFAOYSA-N
Formula:	C6H2Cl5N
SMILES:	Nc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	265.35
CAS:	527-20-8

Physical Properties

Property code	Value	Unit	Source
gf	70.70	kJ/mol	Joback Method
hf	-32.90	kJ/mol	Joback Method
hfus	29.57	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.536		Crippen Method
mcvol	142.820	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	647.94	K	Joback Method
tc	906.88	K	Joback Method
tf	507.06 ± 0.20	K	NIST Webbook
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.19	J/mol×K	820.57	Joback Method

cpg	262.96	J/mol×K	863.72	Joback Method
cpg	240.23	J/mol×K	647.94	Joback Method
cpg	245.57	J/mol×K	691.10	Joback Method
cpg	250.50	J/mol×K	734.25	Joback Method
cpg	255.04	J/mol×K	777.41	Joback Method
cpg	266.36	J/mol×K	906.88	Joback Method
hfust	18.70	kJ/mol	505.80	NIST Webbook
hfust	18.70	kJ/mol	505.80	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=C527208&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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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