Nitrapyrin

Other names:	2-Chloro-6-(trichloromethyl)pyridine
	2-Picoline, «alpha»,«alpha»,«alpha»,6-tetrachloro-
	2-Picoline, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,6-tetrachloro-
	Dowco-163
	N-Serve
	N-Serve nitrogen stabilizer
	Pyridine, 2-chloro-6-(trichloromethyl)-
Inchi:	InChI=1S/C6H3Cl4N/c7-5-3-1-2-4(11-5)6(8,9)10/h1-3H
InchiKey:	DCUJJWWUNKIJPH-UHFFFAOYSA-N
Formula:	C6H3Cl4N
SMILES:	Clc1cccc(C(Cl)(Cl)Cl)n1
Mol. weight [g/mol]:	230.91
CAS:	1929-82-4

Physical Properties

Property code	Value	Unit	Source
chl	-2711.00 ± 20.00	kJ/mol	NIST Webbook
chs	-2830.80 ± 1.60	kJ/mol	NIST Webbook
hfl	498.30	kJ/mol	NIST Webbook
hfs	-55.40 ± 1.80	kJ/mol	NIST Webbook
hvap	58.70	kJ/mol	NIST Webbook
log10ws	-3.76		Aqueous Solubility Prediction Method
log10ws	-3.76		Estimated Solubility Method
logp	3.562		Crippen Method
mcvol	130.580	ml/mol	McGowan Method
ss	244.60	J/mol×K	NIST Webbook
tf	339.03 ± 0.20	K	NIST Webbook
tt	337.24 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cps	189.35	J/mol×K	298.15	NIST Webbook
cps	192.09	J/mol×K	297.13	NIST Webbook
hfust	20.30	kJ/mol	164.50	NIST Webbook
hfust	20.30	kJ/mol	337.20	NIST Webbook
hfust	20.30	kJ/mol	337.24	NIST Webbook
hfust	20.30	kJ/mol	337.24	NIST Webbook
sfust	60.19	J/mol×K	337.24	NIST Webbook
sfust	60.19	J/mol×K	337.24	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1929824&Units=SI

Legend

chl: Standard liquid enthalpy of combustion

chs: Standard solid enthalpy of combustion

cps: Solid phase heat capacity

hfl: Liquid phase enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation 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

sfust: Entropy of fusion at a given temperature

ss: Solid phase molar entropy at standard conditions

tf: Normal melting (fusion) point

tt: Triple Point Temperature