2,3,5,6-TETRACHLOROANILINE

Other names: Aniline, 2,3,5,6-tetrachloro-
2,3,5,6-Tetrachloroaniline
Inchi: InChI=1S/C6H3Cl4N/c7-2-1-3(8)5(10)6(11)4(2)9/h1H,11H2
InchiKey: YTDHEFNWWHSXSU-UHFFFAOYSA-N
Formula: C6H3Cl4N
SMILES: Nc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 230.91

Physical Properties

Property code	Value	Unit	Source
hf	-3.10	kJ/mol	Cheméo Relay (1.0)
hfus	25.77	kJ/mol	Joback Method
hsub	86.00 ± 2.00	kJ/mol	NIST Webbook
hvap	74.39	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-3.88		Cheméo Relay (1.0)
logp	3.882		Crippen Method
mcvol	130.580	ml/mol	McGowan Method
tb	569.76	K	Cheméo Relay (1.0)
tf	391.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.74	J/mol×K	605.53	Joback Method
cpg	231.95	J/mol×K	648.05	Joback Method
cpg	237.70	J/mol×K	690.57	Joback Method
cpg	243.02	J/mol×K	733.09	Joback Method
cpg	247.90	J/mol×K	775.61	Joback Method
cpg	252.38	J/mol×K	818.13	Joback Method
cpg	256.46	J/mol×K	860.65	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=C3481207&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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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