

2,5-Dichloro-4-nitroaniline

Other names:	1-Amino-2,5-dichloro-4-nitrobenzene 2,5-dichloro-4-nitrobenzenamine Aniline, 2,5-dichloro-4-nitro- benzenamine, 2,5-dichloro-4-nitro-
Inchi:	InChI=1S/C6H4Cl2N2O2/c7-3-2-6(10(11)12)4(8)1-5(3)9/h1-2H,9H2
InchiKey:	JBXZCPXEYAEMJS-UHFFFAOYSA-N
Formula:	C6H4Cl2N2O2
SMILES:	Nc1cc(Cl)c([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	207.02

Physical Properties

Property code	Value	Unit	Source
hfus	29.12	kJ/mol	Joback Method
hsub	114.30 ± 0.90	kJ/mol	NIST Webbook
hvap	79.00	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-3.56		Cheméo Relay (1.0)
logp	2.484		Crippen Method
mcvol	123.520	ml/mol	McGowan Method
tb	568.51	K	Cheméo Relay (1.0)
tf	376.37	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.51	J/mol×K	948.30	Joback Method
cpg	291.07	J/mol×K	903.17	Joback Method
cpg	286.09	J/mol×K	858.04	Joback Method
cpg	280.54	J/mol×K	812.91	Joback Method
cpg	274.37	J/mol×K	767.79	Joback Method
cpg	267.57	J/mol×K	722.66	Joback Method
cpg	260.08	J/mol×K	677.53	Joback Method
hsubt	113.20 ± 0.60	kJ/mol	363.00	NIST Webbook

psub	4.34e-04	kPa	366.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	5.43e-04	kPa	368.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.88e-04	kPa	358.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.88e-04	kPa	358.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.47e-04	kPa	360.19	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.44e-04	kPa	360.19	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.41e-04	kPa	360.19	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.93e-04	kPa	362.23	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.89e-04	kPa	362.23	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.80e-04	kPa	362.23	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.49e-04	kPa	364.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.57e-04	kPa	364.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.62e-04	kPa	364.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	4.22e-04	kPa	366.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	9.60e-05	kPa	352.27	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines

psub	4.28e-04	kPa	366.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	5.46e-04	kPa	368.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.84e-04	kPa	358.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	5.29e-04	kPa	368.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	6.52e-04	kPa	370.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	6.66e-04	kPa	370.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	6.67e-04	kPa	370.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	7.75e-04	kPa	372.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	7.79e-04	kPa	372.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	7.74e-04	kPa	372.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	9.66e-04	kPa	374.08	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	9.69e-04	kPa	374.08	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	9.53e-04	kPa	374.08	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.54e-04	kPa	356.14	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines

psub	1.53e-04	kPa	356.14	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.51e-04	kPa	356.14	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.25e-04	kPa	354.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.27e-04	kPa	354.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.29e-04	kPa	354.20	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	9.80e-05	kPa	352.27	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.01e-04	kPa	352.27	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines:	https://www.doi.org/10.1016/j.jct.2009.04.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6627345&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature

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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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