

Botran

Other names:	1-amino-2,6-dichloro-4-nitrobenzene 2,6-Dichlor-4-nitroanilin 2,6-Dichloro-4-nitrobenzeneamine 2,6-dichloro-4-nitroaniline 2,6-dichloro-4-nitrobenzenamine 2,6-dichloro-p-nitroaniline 4-Nitroaniline, 2,6-dichloro- 4-nitro-2,6-dichloroaniline Al-50 Allisan Batran Bortran Botran 75B Botran 75W CDNA CNA DCNA DCNA (fungicide) Dichloran (amine fungicide) Ditranyl NSC 218 RD-6584 Resisan U-2069 aniline, 2,6-dichloro-4-nitro- benzenamine, 2,6-dichloro-4-nitro- dichloran dicloran
Inchi:	InChI=1S/C6H4Cl2N2O2/c7-4-1-3(10(11)12)2-5(8)6(4)9/h1-2H,9H2
InchiKey:	BIXZHMJUSMUDOQ-UHFFFAOYSA-N
Formula:	C6H4Cl2N2O2
SMILES:	<chem>Nc1c(Cl)cc([N+](=O)[O-])cc1Cl</chem>
Mol. weight [g/mol]:	207.01
CAS:	99-30-9

Physical Properties

Property code	Value	Unit	Source
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gf	161.30		kJ/mol	Joback Method
hf	26.50		kJ/mol	Joback Method
hfus	29.12		kJ/mol	Joback Method
hsub	109.20 ± 0.90		kJ/mol	NIST Webbook
hvap	69.21		kJ/mol	Joback Method
log10ws	-3.13			Crippen Method
logp	2.484			Crippen Method
mcvol	123.520		ml/mol	McGowan Method
pc	4368.40		kPa	Joback Method
rinpol	1734.00			NIST Webbook
rinpol	1717.00			NIST Webbook
rinpol	1731.00			NIST Webbook
rinpol	1716.00			NIST Webbook
rinpol	1723.00			NIST Webbook
ripol	2854.00			NIST Webbook
tb	677.53		K	Joback Method
tc	948.30		K	Joback Method
tf	466.80 ± 0.20		K	NIST Webbook
tf	467.44 ± 0.20		K	NIST Webbook
vc	0.472		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.08	J/mol×K	677.53	Joback Method
cpg	267.57	J/mol×K	722.66	Joback Method
cpg	274.37	J/mol×K	767.79	Joback Method
cpg	280.54	J/mol×K	812.91	Joback Method
cpg	286.09	J/mol×K	858.04	Joback Method
cpg	291.07	J/mol×K	903.17	Joback Method
cpg	295.51	J/mol×K	948.30	Joback Method
hfust	32.64	kJ/mol	466.80	NIST Webbook
hfust	29.48	kJ/mol	467.20	NIST Webbook
hsubt	108.20 ± 0.60	kJ/mol	355.00	NIST Webbook
psub	2.54e-04	kPa	352.19	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.06e-04	kPa	344.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines

psub	1.04e-04	kPa	344.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.40e-04	kPa	346.18	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.35e-04	kPa	346.18	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.36e-04	kPa	346.18	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.68e-04	kPa	348.14	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.63e-04	kPa	348.14	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.63e-04	kPa	348.14	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.02e-04	kPa	350.16	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.03e-04	kPa	350.16	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.63e-04	kPa	352.19	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.08e-04	kPa	344.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	2.48e-04	kPa	352.19	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.11e-04	kPa	354.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.10e-04	kPa	354.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.11e-04	kPa	354.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines

psub	3.95e-04	kPa	356.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.67e-04	kPa	356.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	3.68e-04	kPa	356.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	4.94e-04	kPa	358.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	4.68e-04	kPa	358.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	4.64e-04	kPa	358.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	5.83e-04	kPa	360.16	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	5.71e-04	kPa	360.16	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	5.53e-04	kPa	360.16	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	7.25e-04	kPa	362.13	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	7.11e-04	kPa	362.13	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	7.10e-04	kPa	362.13	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	8.64e-04	kPa	364.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	8.57e-04	kPa	364.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines

psub	8.31e-04	kPa	364.15	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.07e-03	kPa	366.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.04e-03	kPa	366.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines
psub	1.01e-03	kPa	366.17	Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines

Sources

Solubility and Solution Thermodynamics of 2,6-Dichloro-4-nitroaniline in 12 Pure Solvents at Temperatures from 278.15 to 323.15 K.
Crippen Method:
McGowan Method:

<https://www.doi.org/10.1021/acs.jced.9b00778>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C99309&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Experimental thermochemical study of 2,5- and 2,6-dichloro-4-nitroanilines:

<https://www.doi.org/10.1016/j.jct.2009.04.012>

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
psub:	Sublimation pressure

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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