

Benzenamine, 2,5-dichloro-4-nitro-

Other names:	2,5-Dichloro-4-nitroaniline Aniline, 2,5-dichloro-4-nitro- 1-Amino-2,5-dichloro-4-nitrobenzene 2,5-Dichloro-4-nitrobenzenamine
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:	<chem>Nc1cc(Cl)c([N+](=O)[O-])cc1Cl</chem>
Mol. weight [g/mol]:	207.01
CAS:	6627-34-5

Physical Properties

Property code	Value	Unit	Source
gf	161.30	kJ/mol	Joback Method
hf	26.50	kJ/mol	Joback Method
h _{fus}	29.12	kJ/mol	Joback Method
h _{sub}	114.30 ± 0.90	kJ/mol	NIST Webbook
h _{vap}	69.21	kJ/mol	Joback Method
log ₁₀ w _s	-3.13		Crippen Method
log _p	2.484		Crippen Method
m _{cvol}	123.520	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	677.53	K	Joback Method
tc	948.30	K	Joback Method
tf	508.07	K	Joback Method
vc	0.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
c _{pg}	260.08	J/mol×K	677.53	Joback Method
c _{pg}	267.57	J/mol×K	722.66	Joback Method
c _{pg}	274.37	J/mol×K	767.79	Joback Method
c _{pg}	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
hsubt	113.20 ± 0.60	kJ/mol	363.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6627345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
mconvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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