

1,3-Dichloro-2-nitrobenzene

Inchi:	InChI=1S/C6H3Cl2NO2/c7-4-2-1-3-5(8)6(4)9(10)11/h1-3H
InchiKey:	VITSNECNFNNVQB-UHFFFAOYSA-N
Formula:	C6H3Cl2NO2
SMILES:	O=[N+]([O-])c1c(Cl)cccc1Cl
Mol. weight [g/mol]:	192.00
CAS:	601-88-7

Physical Properties

Property code	Value	Unit	Source
hf	23.32	kJ/mol	Cheméo Relay (1.0)
hfus	24.31	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-3.40		Cheméo Relay (1.0)
logp	2.902		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
tb	528.84	K	Cheméo Relay (1.0)
tf	345.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	2.34000e+01
Coeff. B	4.88860e-01
Coeff. C	-3.18920e-04
Coeff. D	7.37000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Sources

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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

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