2,4-DICHLORO-1-NITROBENZENE

Other names: 1,3-dichloro-4-nitrobenzene
2,4-dichloronitrobenzene
Benzene, 1,3-dichloro-4-nitro
Inchi: InChI=1S/C6H3Cl2NO2/c7-4-1-2-6(9(10)11)5(8)3-4/h1-3H
InchiKey: QUIMTLZDMCNYGY-UHFFFAOYSA-N
Formula: C6H3Cl2NO2
SMILES: O=[N+]([O-])c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 192.00

Physical Properties

Property code	Value	Unit	Source
hf	14.60	kJ/mol	Cheméo Relay (1.0)
hfus	24.31	kJ/mol	Joback Method
hsub	87.80 ± 1.70	kJ/mol	NIST Webbook
hvap	68.84	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-3.58		Cheméo Relay (1.0)
logp	2.902		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2064.00		NIST Webbook
tb	531.70	K	NIST Webbook
tf	305.00 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.83	J/mol×K	600.02	Joback Method
cpg	225.66	J/mol×K	644.09	Joback Method
cpg	232.80	J/mol×K	688.17	Joback Method

cpg	239.30	J/mol×K	732.24	Joback Method
cpg	245.19	J/mol×K	776.31	Joback Method
cpg	250.50	J/mol×K	820.39	Joback Method
cpg	255.28	J/mol×K	864.46	Joback Method
hvapt	87.80	kJ/mol	298.15	Experimental and computational thermochemical study of the dichloronitrobenzene isomers

Sources

Cheméo Relay (1.0, beta):

Experimental and computational thermochemical study of the dichloronitrobenzene isomers:	https://www.doi.org/10.1016/j.jct.2009.03.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611063&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point