

Benzene, 2,4-dichloro-1-nitro-

Other names:	2,4-Dichloro-1-nitrobenzene 2,4-Dichloronitrobenzene 1,3-Dichloro-4-nitrobenzene 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
CAS:	611-06-3

Physical Properties

Property code	Value	Unit	Source
gf	104.48	kJ/mol	Joback Method
hf	4.18	kJ/mol	Joback Method
hfus	24.31	kJ/mol	Joback Method
hsub	87.80 ± 1.70	kJ/mol	NIST Webbook
hvap	57.91	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.902		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
pc	4135.61	kPa	Joback 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
tc	864.46	K	Joback Method
tf	305.00 ± 1.50	K	NIST Webbook
vc	0.444	m ³ /kmol	Joback Method

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
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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