Chlornitrofen

Other names: Benzene, 1,3,5-trichloro-2-(4-nitrophenoxy)-
Ether, p-nitrophenyl 2,4,6-trichlorophenyl
p-Nitrophenyl 2,4,6-trichlorophenyl ether
CNP
CNP 1032
MC 1478
MO 338
2,4,6-Trichloro-4'-nitrodiphenyl ether
2,4,6-Trichlorophenyl 4-nitrophenyl ether
MC 338
MO
2',4',6'-Trichloro-4-nitrobiphenyl ether
2,4,6-Trichlorophenyl p-nitrophenyl ether
1,3,5-Trichloro-2-(4-nitrophenoxy)benzene
1-Nitro-4-(2,4,6-trichlorophenoxy)benzene
Diphenyl ether, 2,4,6-trichloro-4'-nitro
4-Nitrophenyl 2,4,6-trichlorophenyl ether
Chlomitrofen

Inchi: InChI=1S/C12H6Cl3NO3/c13-7-5-10(14)12(11(15)6-7)19-9-3-1-8(2-4-9)16(17)18/h1-6H

InchiKey: XQNAUQUKWRBODG-UHFFFAOYSA-N

Formula: C12H6Cl3NO3

SMILES: O=[N+]([O-])c1ccc(Oc2c(Cl)cc(Cl)cc2Cl)cc1

Mol. weight [g/mol]: 318.54

CAS: 1836-77-7

Physical Properties

Property code	Value	Unit	Source
gf	131.22	kJ/mol	Joback Method
hf	-54.03	kJ/mol	Joback Method
hfus	38.50	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.347		Crippen Method
mcvol	192.430	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook

rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
rinpol	2342.00		NIST Webbook
rinpol	2326.00		NIST Webbook
ripol	3400.00		NIST Webbook
ripol	3400.00		NIST Webbook
tb	833.79	K	Joback Method
tc	1109.46	K	Joback Method
tf	583.52	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.22	J/mol×K	833.79	Joback Method
cpg	460.20	J/mol×K	879.74	Joback Method
cpg	468.11	J/mol×K	925.68	Joback Method
cpg	474.99	J/mol×K	971.63	Joback Method
cpg	480.89	J/mol×K	1017.57	Joback Method
cpg	485.85	J/mol×K	1063.52	Joback Method
cpg	489.91	J/mol×K	1109.46	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=C1836777&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
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