

Benzene, 1-chloro-4-(4-nitrophenoxy)-

Other names:	p-Chlorophenyl p-nitrophenyl ether Ether, p-chlorophenyl p-nitrophenyl Ether, 4-chlorophenyl 4-nitrophenyl 4'-Chloro-4-nitrobiphenyl ether 1-Chloro-4-(4-nitrophenoxy)benzene
Inchi:	InChI=1S/C12H8ClNO3/c13-9-1-5-11(6-2-9)17-12-7-3-10(4-8-12)14(15)16/h1-8H
InchiKey:	GDEZSMXXDMVYHT-UHFFFAOYSA-N
Formula:	C12H8ClNO3
SMILES:	O=[N+]([O-])c1ccc(Oc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	249.65
CAS:	1836-74-4

Physical Properties

Property code	Value	Unit	Source
gf	174.34	kJ/mol	Joback Method
hf	0.39	kJ/mol	Joback Method
hfus	30.89	kJ/mol	Joback Method
hvap	71.57	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.040		Crippen Method
mcvol	167.950	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	748.97	K	Joback Method
tc	1021.15	K	Joback Method
tf	498.64	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.27	J/molxK	748.97	Joback Method
cpg	429.04	J/molxK	794.33	Joback Method
cpg	439.61	J/molxK	839.70	Joback Method
cpg	449.05	J/molxK	885.06	Joback Method

cpg	457.42	J/mol×K	930.42	Joback Method
cpg	464.76	J/mol×K	975.79	Joback Method
cpg	471.15	J/mol×K	1021.15	Joback Method

Sources

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=C1836744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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