Ether, p-chlorophenyl p-nitrophenyl

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

Physical Properties

Property code	Value	Unit	Source
hf	-21.80	kJ/mol	Cheméo Relay (1.0)
hfus	30.89	kJ/mol	Joback Method
hvap	95.91	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-5.00		Cheméo Relay (1.0)
logp	4.040		Crippen Method
mcvol	167.950	ml/mol	McGowan Method
tb	618.93	K	Cheméo Relay (1.0)
tf	367.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1836744&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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