Benzene, 1-nitro-3-phenoxy-

Other names:	m-Nitrodiphenyl ether
	m-Nitrophenyl phenyl ether
	Ether, m-nitrophenyl phenyl
	3-Nitrodiphenyl ether
	1-nitro-3-phenoxybenzene
Inchi:	InChI=1S/C12H9NO3/c14-13(15)10-5-4-8-12(9-10)16-11-6-2-1-3-7-11/h1-9H
InchiKey:	MEYCCIQOLYYNLD-UHFFFAOYSA-N
Formula:	C12H9NO3
SMILES:	O=[N+]([O-])c1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	215.20
CAS:	620-55-3

Physical Properties

Property code	Value	Unit	Source
gf	195.90	kJ/mol	Joback Method
hf	27.60	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.387		Crippen Method
mcvol	155.710	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
tb	706.56	K	Joback Method
tc	976.45	K	Joback Method
tf	456.20	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.49	J/mol×K	706.56	Joback Method
cpg	410.79	J/mol×K	751.54	Joback Method
cpg	422.81	J/mol×K	796.52	Joback Method
cpg	433.62	J/mol×K	841.51	Joback Method

cpg	443.29	J/mol×K	886.49	Joback Method
cpg	451.88	J/mol×K	931.47	Joback Method
cpg	459.47	J/mol×K	976.45	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=C620553&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