

Benzene, 1-nitro-2-phenoxy-

Other names:	o-Nitrophenyl phenyl ether o-Nitro diphenyl ether Ether, o-nitrophenyl phenyl Ether, 2-nitrophenyl phenyl Phenyl o-nitrophenyl ether 1-Nitro-2-phenoxybenzene 2-Nitrodiphenyl ether 2-Nitrophenyl phenyl ether 2-NDE Ether, 2-nitrodiphenyl, 2-Phenoxy nitrobenzene
Inchi:	InChI=1S/C12H9NO3/c14-13(15)11-8-4-5-9-12(11)16-10-6-2-1-3-7-10/h1-9H
InchiKey:	VNHGETRQQSYUGZ-UHFFFAOYSA-N
Formula:	C12H9NO3
SMILES:	O=[N+]([O-])c1ccccc1Oc1ccccc1
Mol. weight [g/mol]:	215.20
CAS:	2216-12-8

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.49	J/molxK	706.56	Joback Method
cpg	410.79	J/molxK	751.54	Joback Method
cpg	422.81	J/molxK	796.52	Joback Method
cpg	433.62	J/molxK	841.51	Joback Method
cpg	443.29	J/molxK	886.49	Joback Method
cpg	451.88	J/molxK	931.47	Joback Method
cpg	459.47	J/molxK	976.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	508.20	K	8.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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