2-NITROPHENYL ISOCYANATE

Other names:	o-Nitrophenyl isocyanate
	Benzene, 1-isocyanato-2-nitro-
	Isocyanic acid, o-nitrophenyl ester
Inchi:	InChI=1S/C7H4N2O3/c10-5-8-6-3-1-2-4-7(6)9(11)12/h1-4H
InchiKey:	JRVZITODZAQRQM-UHFFFAOYSA-N
Formula:	C7H4N2O3
SMILES:	O=C=Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	164.12

Physical Properties

Property code	Value	Unit	Source
hf	46.66	kJ/mol	Cheméo Relay (1.0)
hvap	62.55	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-2.75		Cheméo Relay (1.0)
logp	1.562		Crippen Method
mcvol	110.400	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
tb	520.66	K	Cheméo Relay (1.0)
tc	779.81	K	Cheméo Relay (1.0)
tf	327.17	K	Cheméo Relay (1.0)

Sources

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=C3320863&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation 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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point