Benzene, 1-isothiocyanato-3-nitro-

Other names:	Isothiocyanic acid, m-nitrophenyl ester
	m-Nitrophenyl isothiocyanate
	3-Nitrophenyl isothiocyanate
	Phenyl, 3-nitro, isothiocyanate
	Phenylisothiocyanate, 3-nitro
Inchi:	InChI=1S/C7H4N2O2S/c10-9(11)7-3-1-2-6(4-7)8-5-12/h1-4H
InchiKey:	OEZXLKSZOAWNJU-UHFFFAOYSA-N
Formula:	C7H4N2O2S
SMILES:	O=[N+]([O-])c1cccc(N=C=S)c1
Mol. weight [g/mol]:	180.18
CAS:	3529-82-6

Physical Properties

Property code	Value	Unit	Source
hf	310.56	kJ/mol	Joback Method
hvap	61.15	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.329		Crippen Method
mcvol	120.880	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	689.01	K	Joback Method
tc	980.14	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C3529826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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