Benzene, 1-nitro-4-(phenylthio)-

Other names:	Sulfide, p-nitrophenyl phenyl
	p-Nitrodiphenyl sulfide
	p-Nitrophenyl phenyl sulfide
	Phenyl p-nitrophenylsulfide
	4-Nitrodiphenyl sulfide
	4-Nitrophenyl phenyl sulfide
	4-(Phenylthio)nitrobenzene
	1-Nitro-4-(phenylsulfanyl)benzene
	1-Nitro-4-(phenylthio)benzene
	NSC 87341
	4-nitrophenyl phenyl sulphide
Inchi:	InChI=1S/C12H9NO2S/c14-13(15)10-6-8-12(9-7-10)16-11-4-2-1-3-5-11/h1-9H
InchiKey:	RJCBYBQJVXVVKB-UHFFFAOYSA-N
Formula:	C12H9NO2S
SMILES:	O=[N+]([O-])c1ccc(Sc2ccccc2)cc1
Mol. weight [g/mol]:	231.27
CAS:	952-97-6

Physical Properties

Property code	Value	Unit	Source
gf	334.02	kJ/mol	Joback Method
hf	201.69	kJ/mol	Joback Method
hfus	30.02	kJ/mol	Joback Method
hvap	70.93	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.746		Crippen Method
mcvol	166.190	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	752.92	K	Joback Method
tc	1044.88	K	Joback Method
tf	468.37	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.11	J/mol×K	752.92	Joback Method
cpg	432.86	J/mol×K	801.58	Joback Method
cpg	444.18	J/mol×K	850.24	Joback Method
cpg	454.18	J/mol×K	898.90	Joback Method
cpg	462.95	J/mol×K	947.56	Joback Method
cpg	470.60	J/mol×K	996.22	Joback Method
cpg	477.23	J/mol×K	1044.88	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	561.40	K	13.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C952976&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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