Bis(4-nitrophenyl)disulfide

Other names: 4-Nitrophenyl disulfide
4,4'-Dinitrodiphenyl disulfide
Disulfide, bis(4-nitrophenyl)
p-Nitrophenyl disulfide
p,p'-Dinitrodiphenyl disulfide
Bis(p-nitrophenyl) disulfide
Di(p-nitrophenyl) disulfide
Di-4-nitrophenyl disulfide
Disulfide, bis(p-nitrophenyl)
NSC 677446
1-Nitro-4-[(4-nitrophenyl)disulfanyl]benzene
NSC 4566
bis(4-nitrophenyl) disulphide
Di-4-nitrophenyl sulfide

Inchi: InChI=1S/C12H8N2O4S2/c15-13(16)9-1-5-11(6-2-9)19-20-12-7-3-10(4-8-12)14(17)18/h1

InchiKey: KWGZRLZJBLEVFZ-UHFFFAOYSA-N

Formula: C12H8N2O4S2

SMILES: O=[N+]([O-])c1ccc(SSc2ccc([N+](=O)[O-])cc2)cc1

Mol. weight [g/mol]: 308.33

CAS: 100-32-3

Physical Properties

Property code	Value	Unit	Source
gf	393.06	kJ/mol	Joback Method
hf	221.33	kJ/mol	Joback Method
hfus	45.12	kJ/mol	Joback Method
hvap	95.00	kJ/mol	Joback Method
ie	8.98	eV	NIST Webbook
log10ws	-6.06		Crippen Method
logp	4.302		Crippen Method
mcvol	199.960	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	978.52	K	Joback Method
tc	1295.96	K	Joback Method
tf	658.90	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.82	J/mol×K	978.52	Joback Method
cpg	545.01	J/mol×K	1031.43	Joback Method
cpg	550.69	J/mol×K	1084.33	Joback Method
cpg	554.95	J/mol×K	1137.24	Joback Method
cpg	557.90	J/mol×K	1190.15	Joback Method
cpg	559.65	J/mol×K	1243.05	Joback Method
cpg	560.29	J/mol×K	1295.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100323&Units=SI

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
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

vc: Critical Volume