

BIS(P-NITROPHENYL) SULFIDE

Other names:	4,4'-Dinitrodiphenylsulphide 4-Nitrophenyl sulfide p-Nitrophenyl sulfide Benzene, 1,1'-thiobis[4-nitro- p,p'-Dinitrodiphenyl sulfide Bis(p-nitrophenyl)sulfide Bis(4-nitrophenyl)sulfide Sulfide, bis(p-nitrophenyl) 4,4'-Dinitrodiphenyl sulfide NSC 11350 bis(4-nitrophenyl) sulphide
Inchi:	InChI=1S/C12H8N2O4S/c15-13(16)9-1-5-11(6-2-9)19-12-7-3-10(4-8-12)14(17)18/h1-8H
InchiKey:	ZZTJMQPRKBNGNX-UHFFFAOYSA-N
Formula:	C12H8N2O4S
SMILES:	O=[N+]([O-])c1ccc(Sc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	276.27

Physical Properties

Property code	Value	Unit	Source
hf	170.93	kJ/mol	Cheméo Relay (1.0)
hfus	40.99	kJ/mol	Joback Method
hvap	112.83	kJ/mol	Cheméo Relay (1.0)
ie	8.86	eV	Cheméo Relay (1.0)
log10ws	-5.36		Cheméo Relay (1.0)
logp	3.654		Crippen Method
mcvol	183.610	ml/mol	McGowan Method
tb	653.15	K	Cheméo Relay (1.0)
tf	432.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.04	J/mol×K	909.74	Joback Method
cpg	508.17	J/mol×K	960.55	Joback Method

cpg	515.98	J/mol×K	1011.36	Joback Method
cpg	522.57	J/mol×K	1062.17	Joback Method
cpg	528.06	J/mol×K	1112.99	Joback Method
cpg	532.57	J/mol×K	1163.80	Joback Method
cpg	536.22	J/mol×K	1214.61	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1223310&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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