BIS(P-NITROPHENYL) ETHER

Other names:	4,4'-Dinitrodiphenyl ether
	Benzene, 1,1'-oxybis[4-nitro-
	p-Nitrophenyl ether
	p,p'-Dinitrodiphenyl ether
	Bis(4-nitrophenyl) ether
	Di-4-nitrophenyl ether
	Ether, bis(p-nitrophenyl)
	Ether, bis(4-nitrophenyl)
	Oxybis(4-nitrobenzene)
	4,4'-Dinitrodiphenyl oxide
	NSC 8740
Inchi:	InChI=1S/C12H8N2O5/c15-13(16)9-1-5-11(6-2-9)19-12-7-3-10(4-8-12)14(17)18/h1-8H
InchiKey:	MWAGUKZCDDRDCS-UHFFFAOYSA-N
Formula:	C12H8N2O5
SMILES:	O=[N+]([O-])c1ccc(Oc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	260.20

Physical Properties

Property code	Value	Unit	Source
hf	12.14	kJ/mol	Cheméo Relay (1.0)
hfus	38.05	kJ/mol	Joback Method
hvap	105.36	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
log10ws	-4.70		Cheméo Relay (1.0)
logp	3.295		Crippen Method
mcvol	173.130	ml/mol	McGowan Method
tb	619.59	K	Cheméo Relay (1.0)
tf	418.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.91	J/mol×K	863.38	Joback Method
cpg	490.91	J/mol×K	910.96	Joback Method

cpg	499.63	J/mol×K	958.53	Joback Method
cpg	507.15	J/mol×K	1006.11	Joback Method
cpg	513.55	J/mol×K	1053.68	Joback Method
cpg	518.90	J/mol×K	1101.26	Joback Method
cpg	523.28	J/mol×K	1148.84	Joback Method
cps	421.70	J/mol×K	298.00	NIST Webbook
hfust	10.29	kJ/mol	418.20	NIST Webbook
hfust	10.29	kJ/mol	418.20	NIST Webbook
hfust	10.29	kJ/mol	418.20	NIST Webbook
sfust	24.60	J/mol×K	418.20	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101633&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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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