Phenol, 4-[(2,4-dinitrophenyl)amino]-

Other names:

2,4-Dinitro-4'-hydroxydiphenylamine
2,4-Dinitro-p-hydroxydiphenylamine
4'-Hydroxy-2,4-dinitrodiphenylamine
4-(2,4-Dinitroanilino)phenol
4-Hydroxy-2',4'-dinitrodiphenylamine
4-[(2,4-Dinitrophenyl)amino]phenol
Acetamine Yellow 2R
Acetoquinone Light Yellow 2RZ
Amacel Yellow RR
C.I. 10345
C.I. Disperse Yellow 1
C.I. Solvent Yellow 52
Celliton Fast Yellow RR
Celliton Fast Yellow RRA-CF
Cilla Fast Yellow RR
Disperse Fast Yellow 2K
Disperse Yellow R
Disperse yellow stable 2K
Dispersol Fast Yellow A
Dispersol Printing Yellow A
Dispersol yellow B-A
Fast Disperse Yellow 2K
Fenacet Fast Yellow 2R
Kayalon Fast Yellow RR
Microsetile Yellow 2R
N-(2,4-Dinitrophenyl)-N-(4-hydroxyphenyl)amine
N-2,4-Dinitrophenyl-4-aminophenol
NSC 13965
Nyloquinone Yellow 2R
Perliton Yellow RR
Permanent Yellow 2K
Phenol, 4-[(2,4-dinitrophenyl)amino]-
Phenol, p-(2,4-dinitroanilino)-
Reliton Yellow R
SRA Golden Yellow VIII
Serisol Fast Yellow A
Setacyl Yellow P-BS
Supracet Fast Yellow 2R
Supracet Yellow RR
Synten yellow P 2R

	p-(2,4-Dinitroanilino)phenol
Inchi:	InChI=1S/C12H9N3O5/c16-10-4-1-8(2-5-10)13-11-6-3-9(14(17)18)7-12(11)15(19)20/h1-
InchiKey:	BCPQALWAROJVLE-UHFFFAOYSA-N
Formula:	C12H9N3O5
SMILES:	O=[N+]([O-])c1ccc(Nc2ccc(O)cc2)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	275.22

Physical Properties

Property code	Value	Unit	Source
hf	10.56	kJ/mol	Cheméo Relay (1.0)
hfus	47.74	kJ/mol	Joback Method
hvap	120.52	kJ/mol	Cheméo Relay (1.0)
ie	7.74	eV	Cheméo Relay (1.0)
log10ws	-3.78		Cheméo Relay (1.0)
logp	2.952		Crippen Method
mcvol	183.110	ml/mol	McGowan Method
tb	665.44	K	Cheméo Relay (1.0)
tf	463.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.17	J/mol×K	971.75	Joback Method
cpg	551.10	J/mol×K	1019.70	Joback Method
cpg	560.79	J/mol×K	1067.65	Joback Method
cpg	570.45	J/mol×K	1115.60	Joback Method
cpg	580.29	J/mol×K	1163.55	Joback Method
cpg	590.52	J/mol×K	1211.50	Joback Method
cpg	601.34	J/mol×K	1259.45	Joback Method
hsubt	155.60 ± 4.20	kJ/mol	455.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119153&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
hsubt:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point