Benzenamine, 2,4-dinitro-N-phenyl-

Other names:	Diphenylamine, 2,4-dinitro- o,p-Dinitrodiphenylamine Acetoquinone Yellow 5JZ C.I. Disperse Yellow 14 C.I. 10340 N-(2,4-Dinitrophenyl)aniline Serisol Yellow 2G Supracet Yellow 3G 2,4-Dinitrodiphenylamine N-Phenyl-2,4-dinitroaniline NSC 6150 2,4-dinitro-N-phenylaniline
Inchi:	InChI=1S/C12H9N3O4/c16-14(17)10-6-7-11(12(8-10)15(18)19)13-9-4-2-1-3-5-9/h1-8,13H
InchiKey:	RHTVQEPJVKUMPI-UHFFFAOYSA-N
Formula:	C12H9N3O4
SMILES:	O=[N+]([O-])c1ccc(Nc2ccccc2)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	259.22
CAS:	961-68-2

Physical Properties

Property code	Value	Unit	Source
chs	-6030.80 ± 5.90	kJ/mol	NIST Webbook
gf	416.21	kJ/mol	Joback Method
hf	191.06	kJ/mol	Joback Method
hfs	22.50 ± 5.90	kJ/mol	NIST Webbook
hfus	41.96	kJ/mol	Joback Method
hvap	87.80	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.247		Crippen Method
mcvol	177.240	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	891.13	K	Joback Method
tc	1175.86	K	Joback Method
tf	642.76	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.71	J/mol×K	1080.95	Joback Method
cpg	542.71	J/mol×K	1128.40	Joback Method
cpg	503.88	J/mol×K	891.13	Joback Method
cpg	513.65	J/mol×K	938.58	Joback Method
cpg	522.29	J/mol×K	986.04	Joback Method
cpg	529.94	J/mol×K	1033.49	Joback Method
cpg	548.06	J/mol×K	1175.86	Joback Method
hsubt	147.60	kJ/mol	411.00	NIST Webbook
hsubt	156.60	kJ/mol	448.50	NIST Webbook

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=C961682&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
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