Benzenamine, 2-nitro-N-(4-nitrophenyl)-

Other names: Diphenylamine, 2,4'-dinitro-
2,4'-Dinitrodiphenylamine
2-nitro-N-(4-nitrophenyl)aniline
Inchi: InChI=1S/C12H9N3O4/c16-14(17)10-7-5-9(6-8-10)13-11-3-1-2-4-12(11)15(18)19/h1-8,13
InchiKey: TXJIDOLTOGSNPD-UHFFFAOYSA-N
Formula: C12H9N3O4
SMILES: O=[N+]([O-])c1ccc(Nc2ccccc2[N+](=O)[O-])cc1
Mol. weight [g/mol]: 259.22
CAS: 612-36-2

Physical Properties

Property code	Value	Unit	Source
gf	416.21	kJ/mol	Joback Method
hf	191.06	kJ/mol	Joback Method
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	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	536.71	J/mol×K	1080.95	Joback Method
cpg	542.71	J/mol×K	1128.40	Joback Method

cpg	548.06	J/mol×K	1175.86	Joback Method

Sources

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=C612362&Units=SI
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
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
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