2,4-dinitrodiphenylamine

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

Physical Properties

Property code	Value	Unit	Source
gf	416.21	kJ/mol	Joback Method
hf	191.06	kJ/mol	Joback Method
hfus	14.37	kJ/mol	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
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	431.35	K	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures:	https://www.doi.org/10.1016/j.jct.2010.03.025

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