(4-Nitrophenyl)diphenylamine

Other names: p-nitrotriphenylamine
Inchi: InChI=1S/C18H14N2O2/c21-20(22)18-13-11-17(12-14-18)19(15-7-3-1-4-8-15)16-9-5-2-6
InchiKey: UQOKZDUUBVGFAK-UHFFFAOYSA-N
Formula: C18H14N2O2
SMILES: O=[N+]([O-])c1ccc(N(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 290.32
CAS: 4316-57-8

Physical Properties

Property code	Value	Unit	Source
gf	574.61	kJ/mol	Joback Method
hf	340.04	kJ/mol	Joback Method
hfus	38.49	kJ/mol	Joback Method
hvap	81.79	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.065		Crippen Method
mcvol	220.600	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
tb	860.54	K	Joback Method
tc	1140.76	K	Joback Method
tf	560.48	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.02	J/mol×K	860.54	Joback Method
cpg	649.95	J/mol×K	907.24	Joback Method
cpg	662.47	J/mol×K	953.95	Joback Method
cpg	673.76	J/mol×K	1000.65	Joback Method
cpg	684.02	J/mol×K	1047.35	Joback Method
cpg	693.43	J/mol×K	1094.06	Joback Method
cpg	702.20	J/mol×K	1140.76	Joback Method

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=C4316578&Units=SI

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