(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

Physical Properties

Property code	Value	Unit	Source
hf	287.25	kJ/mol	Cheméo Relay (1.0)
hfus	38.49	kJ/mol	Joback Method
hvap	109.11	kJ/mol	Cheméo Relay (1.0)
ie	7.29	eV	Cheméo Relay (1.0)
log10ws	-5.31		Cheméo Relay (1.0)
logp	5.065		Crippen Method
mcvol	220.600	ml/mol	McGowan Method
tb	683.80	K	Cheméo Relay (1.0)
tf	414.43	K	Cheméo Relay (1.0)

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

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4316578&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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