NITROBENZENE, 4-(2-CYANO-2-PHENYLETHENYL)

Inchi: InChI=1S/C15H10N2O2/c16-11-14(13-4-2-1-3-5-13)10-12-6-8-15(9-7-12)17(18)19/h1-10

InchiKey: WWCOVEKFRJZIDP-GXDHUFHOSA-N

Formula: C15H10N2O2

SMILES: N#C/C(=C\c1ccc([N+](=O)[O-])cc1)c1ccccc1

Mol. weight [g/mol]: 250.26

Physical Properties

Property code	Value	Unit	Source
chs	-7490.00	kJ/mol	NIST Webbook
hf	366.27	kJ/mol	Cheméo Relay (1.0)
hfs	155.00	kJ/mol	NIST Webbook
hfus	34.06	kJ/mol	Joback Method
hvap	98.32	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-4.99		Cheméo Relay (1.0)
logp	3.659		Crippen Method
mcvol	189.190	ml/mol	McGowan Method
tb	653.83	K	Cheméo Relay (1.0)
tf	433.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.14	J/mol×K	858.90	Joback Method
cpg	525.21	J/mol×K	905.26	Joback Method
cpg	535.30	J/mol×K	951.63	Joback Method
cpg	544.57	J/mol×K	997.99	Joback Method
cpg	553.19	J/mol×K	1044.36	Joback Method
cpg	561.29	J/mol×K	1090.72	Joback Method
cpg	569.03	J/mol×K	1137.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7431358&Units=SI
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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