

Nitrobenzene, 3-(2-cyano-2-phenylethenyl)

Inchi: InChI=1S/C15H10N2O2/c16-11-14(13-6-2-1-3-7-13)9-12-5-4-8-15(10-12)17(18)19/h1-10
InchiKey: MHBAKHXYJYROG-ZROIWOOFSA-N
Formula: C15H10N2O2
SMILES: N#CC(=Cc1cccc([N+](=O)[O-])c1)c1ccccc1
Mol. weight [g/mol]: 250.25
CAS: 6720-37-2

Physical Properties

Property code	Value	Unit	Source
chs	-7504.76	kJ/mol	NIST Webbook
chs	-7508.00	kJ/mol	NIST Webbook
gf	531.01	kJ/mol	Joback Method
hf	370.21	kJ/mol	Joback Method
hfs	172.90	kJ/mol	NIST Webbook
hfs	176.00	kJ/mol	NIST Webbook
hfus	34.06	kJ/mol	Joback Method
h vap	81.30	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.659		Crippen Method
m cvol	189.190	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	858.90	K	Joback Method
tc	1137.09	K	Joback Method
tf	513.73	K	Joback Method
vc	0.749	m ³ /kmol	Joback Method

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

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=C6720372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
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

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