Cyclopropanecarbonitrile, 1-(p-nitrophenyl)-2-phenyl-

Inchi: InChI=1S/C16H12N2O2/c17-11-16(10-15(16)12-4-2-1-3-5-12)13-6-8-14(9-7-13)18(19)20

InchiKey: AVYTZYMHDAMJRD-UHFFFAOYSA-N

Formula: C16H12N2O2

SMILES: N#CC1(c2ccc([N+](=O)[O-])cc2)CC1c1ccccc1

Mol. weight [g/mol]: 264.28

CAS: 10432-22-1

Physical Properties

Property code	Value	Unit	Source
gf	515.31	kJ/mol	Joback Method
hf	309.84	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	81.95	kJ/mol	Joback Method
ie	9.05 ± 0.10	eV	NIST Webbook
log10ws	-4.78		Crippen Method
logp	3.544		Crippen Method
mcvol	196.720	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	880.05	K	Joback Method
tc	1163.72	K	Joback Method
tf	581.64	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.02	J/mol×K	880.05	Joback Method
cpg	596.61	J/mol×K	927.33	Joback Method
cpg	612.42	J/mol×K	974.61	Joback Method
cpg	628.82	J/mol×K	1021.88	Joback Method
cpg	646.18	J/mol×K	1069.16	Joback Method
cpg	664.88	J/mol×K	1116.44	Joback Method
cpg	685.28	J/mol×K	1163.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10432221&Units=SI
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

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
ie:	Ionization energy
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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