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

Inchi: InChI=1S/C16H11N3O4/c17-10-16(12-3-7-14(8-4-12)19(22)23)9-15(16)11-1-5-13(6-2-11
InchiKey: QMOQSTMQXUSYQB-UHFFFAOYSA-N
Formula: C16H11N3O4
SMILES: N#CC1(c2ccc([N+](=O)[O-])cc2)CC1c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 309.28
CAS: 28752-28-5

Physical Properties

Property code	Value	Unit	Source
gf	541.23	kJ/mol	Joback Method
hf	287.61	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	99.20	kJ/mol	Joback Method
ie	9.30 ± 0.05	eV	NIST Webbook
log10ws	-5.43		Crippen Method
logp	3.452		Crippen Method
mcvol	214.140	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
tb	1036.87	K	Joback Method
tc	1332.27	K	Joback Method
tf	737.77	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.42	J/mol×K	1036.87	Joback Method
cpg	695.85	J/mol×K	1086.10	Joback Method
cpg	715.75	J/mol×K	1135.34	Joback Method
cpg	737.52	J/mol×K	1184.57	Joback Method
cpg	761.58	J/mol×K	1233.80	Joback Method
cpg	788.35	J/mol×K	1283.04	Joback Method
cpg	818.25	J/mol×K	1332.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28752285&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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