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

Inchi: InChI=1S/C16H12ClN/c17-14-8-6-13(7-9-14)16(11-18)10-15(16)12-4-2-1-3-5-12/h1-9,15

InchiKey: WNUOJHANAJTNCJ-UHFFFAOYSA-N

Formula: C16H12ClN

SMILES: N#CC1(c2ccc(Cl)cc2)CC1c1ccccc1

Mol. weight [g/mol]: 253.73

CAS: 32589-55-2

Physical Properties

Property code	Value	Unit	Source
gf	467.83	kJ/mol	Joback Method
hf	304.86	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
ie	8.18 ± 0.10	eV	NIST Webbook
log10ws	-4.81		Crippen Method
logp	4.289		Crippen Method
mcvol	191.540	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	765.64	K	Joback Method
tc	1036.33	K	Joback Method
tf	467.95	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.61	J/mol×K	765.64	Joback Method
cpg	522.51	J/mol×K	810.76	Joback Method
cpg	536.91	J/mol×K	855.87	Joback Method
cpg	551.11	J/mol×K	900.99	Joback Method
cpg	565.44	J/mol×K	946.10	Joback Method
cpg	580.21	J/mol×K	991.22	Joback Method
cpg	595.75	J/mol×K	1036.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32589552&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