BENZENE, 1-CHLORO-4-(2-CYANO-2-PHENYLETHENYL)

Other names: p-Chloro-«alpha»-phenylcinnamonitrile
Acrylonitrile, 3-(p-chlorophenyl)-2-phenyl-
Benzeneacetonitrile, «alpha»-((4-chlorophenyl)methylene)-
4-Chlor-benzal-(benzyl-cyanid)
3-(p-Chlorophenyl)-2-phenylacrylonitrile
F 2388
3-(4-Chlorophenyl)-2-phenyl-2-propenenitrile

Inchi: InChI=1S/C15H10ClN/c16-15-8-6-12(7-9-15)10-14(11-17)13-4-2-1-3-5-13/h1-10H/b14-1

InchiKey: WHZUHCZQGFNGNH-GXDHUFHOSA-N

Formula: C15H10ClN

SMILES: N#C/C(=C\c1ccc(Cl)cc1)c1ccccc1

Mol. weight [g/mol]: 239.71

Physical Properties

Property code	Value	Unit	Source
hf	346.89	kJ/mol	Cheméo Relay (1.0)
hfus	26.89	kJ/mol	Joback Method
ie	8.50	eV	Cheméo Relay (1.0)
logp	4.404		Crippen Method
mcvol	184.010	ml/mol	McGowan Method
tb	638.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.90	J/mol×K	744.49	Joback Method
cpg	460.36	J/mol×K	788.59	Joback Method
cpg	471.71	J/mol×K	832.69	Joback Method
cpg	482.09	J/mol×K	876.79	Joback Method
cpg	491.62	J/mol×K	920.88	Joback Method
cpg	500.43	J/mol×K	964.98	Joback Method
cpg	508.65	J/mol×K	1009.08	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3695929&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):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature