

Benzene, 1-chloro-4-(2-cyano-2-phenylethenyl)

Other names:	p-Chloro-«alpha»-phenylcinnamionitrile 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/b14-10
InchiKey:	WHZUHCZQGFNGNH-GXDHUFHOSA-N
Formula:	C15H10ClN
SMILES:	N#CC(=Cc1ccc(Cl)cc1)c1ccccc1
Mol. weight [g/mol]:	239.70
CAS:	3695-92-9

Physical Properties

Property code	Value	Unit	Source
gf	483.53	kJ/mol	Joback Method
hf	365.23	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.404		Crippen Method
mcvol	184.010	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	744.49	K	Joback Method
tc	1009.08	K	Joback Method
tf	400.04	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

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

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=C3695929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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