«alpha»-(p-Chlorophenyl)cinnamonitrile

Other names: Acrylonitrile, 2-(p-chlorophenyl)-3-phenyl-
Benzal-(4'-chlor-benzyl-cyanid)
Benzeneacetonitrile, 4-chloro-«alpha»-(phenylmethylene)-
2-(p-Chlorophenyl)-3-phenylacrylonitrile
F 2389
alpha-(p-Chlorophenyl)cinnamonitrile

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

InchiKey: JJGLLZWUWIKTAG-GXDHUFHOSA-N

Formula: C15H10ClN

SMILES: N#CC(=Cc1ccccc1)c1ccc(Cl)cc1

Mol. weight [g/mol]: 239.70

CAS: 3695-93-0

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	m3/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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3695930&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
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