m-Chlorobenzylidene-p-chlorophenylacetonitrile

Inchi: InChI=1S/C15H9Cl2N/c16-14-6-4-12(5-7-14)13(10-18)8-11-2-1-3-15(17)9-11/h1-9H/b13-
InchiKey: QKPFBKLGLGRHFG-MDWZMJQESA-N
Formula: C15H9Cl2N
SMILES: N#CC(=Cc1cccc(Cl)c1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 274.14
CAS: 93986-80-2

Physical Properties

Property code	Value	Unit	Source
gf	461.97	kJ/mol	Joback Method
hf	338.02	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.058		Crippen Method
mcvol	196.250	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	786.90	K	Joback Method
tc	1053.63	K	Joback Method
tf	442.48	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.75	J/mol×K	786.90	Joback Method
cpg	477.86	J/mol×K	831.36	Joback Method
cpg	488.00	J/mol×K	875.81	Joback Method
cpg	497.29	J/mol×K	920.27	Joback Method
cpg	505.86	J/mol×K	964.72	Joback Method
cpg	513.83	J/mol×K	1009.18	Joback Method
cpg	521.32	J/mol×K	1053.63	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=C93986802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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