m-Chlorobenzylidene-2-methylphenylacetonitrile

Inchi: InChI=1S/C16H12ClN/c1-12-5-2-3-8-16(12)14(11-18)9-13-6-4-7-15(17)10-13/h2-10H,1H
InchiKey: QPOPXCYGXDXKCB-NTEUORMPSA-N
Formula: C16H12ClN
SMILES: Cc1ccccc1C(C#N)=Cc1cccc(Cl)c1
Mol. weight [g/mol]: 253.73
CAS: 31881-10-4

Physical Properties

Property code	Value	Unit	Source
gf	482.32	kJ/mol	Joback Method
hf	333.12	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	71.99	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.713		Crippen Method
mcvol	198.100	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	772.35	K	Joback Method
tc	1031.54	K	Joback Method
tf	423.83	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.28	J/mol×K	772.35	Joback Method
cpg	511.13	J/mol×K	815.55	Joback Method
cpg	522.93	J/mol×K	858.75	Joback Method
cpg	533.79	J/mol×K	901.94	Joback Method
cpg	543.83	J/mol×K	945.14	Joback Method
cpg	553.14	J/mol×K	988.34	Joback Method
cpg	561.86	J/mol×K	1031.54	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=C31881104&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