p-Methoxybenzylidene-p-chlorophenylacetonitrile

Inchi: InChI=1S/C16H12ClNO/c1-19-16-8-2-12(3-9-16)10-14(11-18)13-4-6-15(17)7-5-13/h2-10
InchiKey: VXRHURWDVQKETO-GXDHUFHOSA-N
Formula: C16H12ClNO
SMILES: COc1ccc(C=C(C#N)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 269.73
CAS: 72030-11-6

Physical Properties

Property code	Value	Unit	Source
gf	377.32	kJ/mol	Joback Method
hf	200.90	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.413		Crippen Method
mcvol	203.970	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
tb	794.77	K	Joback Method
tc	1049.59	K	Joback Method
tf	446.06	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.96	J/mol×K	794.77	Joback Method
cpg	535.42	J/mol×K	837.24	Joback Method
cpg	546.81	J/mol×K	879.71	Joback Method
cpg	557.23	J/mol×K	922.18	Joback Method
cpg	566.75	J/mol×K	964.65	Joback Method
cpg	575.46	J/mol×K	1007.12	Joback Method
cpg	583.43	J/mol×K	1049.59	Joback Method

Sources

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/inchi/InChI%3D1S/C16H12ClNO/c1-19-16-8-2-12(3-9-16)10-14(11
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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