m-Nitrobenzylidene-p-isopropylphenylacetonitrile

Inchi: InChI=1S/C18H16N2O2/c1-13(2)15-6-8-16(9-7-15)17(12-19)10-14-4-3-5-18(11-14)20(21
InchiKey: PWWZEFHODWBKGO-LICLKQGHSA-N
Formula: C18H16N2O2
SMILES: CC(C)c1ccc(C(C#N)=Cc2cccc([N+](=O)[O-])c2)cc1
Mol. weight [g/mol]: 292.33
CAS: 53466-03-8

Physical Properties

Property code	Value	Unit	Source
chs	-9506.55	kJ/mol	NIST Webbook
gf	544.20	kJ/mol	Joback Method
hf	291.54	kJ/mol	Joback Method
hfs	136.60	kJ/mol	NIST Webbook
hfus	37.92	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	4.782		Crippen Method
mcvol	231.460	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
tb	932.08	K	Joback Method
tc	1198.17	K	Joback Method
tf	545.06	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.78	J/mol×K	932.08	Joback Method
cpg	691.08	J/mol×K	976.43	Joback Method
cpg	702.44	J/mol×K	1020.78	Joback Method
cpg	713.00	J/mol×K	1065.13	Joback Method
cpg	722.88	J/mol×K	1109.47	Joback Method
cpg	732.25	J/mol×K	1153.82	Joback Method
cpg	741.22	J/mol×K	1198.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53466038&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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