o-Nitrobenzylidene-2-methylphenylacetonitrile

Inchi: InChI=1S/C16H12N2O2/c1-12-6-2-4-8-15(12)14(11-17)10-13-7-3-5-9-16(13)18(19)20/h2
InchiKey: OXSUKILYXSKWSY-GXDHUFHOSA-N
Formula: C16H12N2O2
SMILES: Cc1ccccc1C(C#N)=Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 264.28
CAS: 31881-12-6

Physical Properties

Property code	Value	Unit	Source
chs	-8180.00	kJ/mol	NIST Webbook
gf	529.80	kJ/mol	Joback Method
hf	338.10	kJ/mol	Joback Method
hfs	165.00	kJ/mol	NIST Webbook
hfus	36.26	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.967		Crippen Method
mcvol	203.280	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	886.76	K	Joback Method
tc	1159.23	K	Joback Method
tf	537.52	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.68	J/mol×K	886.76	Joback Method
cpg	578.13	J/mol×K	932.17	Joback Method
cpg	588.63	J/mol×K	977.58	Joback Method
cpg	598.33	J/mol×K	1022.99	Joback Method
cpg	607.36	J/mol×K	1068.40	Joback Method
cpg	615.85	J/mol×K	1113.81	Joback Method
cpg	623.95	J/mol×K	1159.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31881126&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

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