4-Nitrobenzoic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C16H15NO5/c1-11(2)21-14-5-3-4-6-15(14)22-16(18)12-7-9-13(10-8-12)17(19)
InchiKey: QBOHGJVUEGQPDY-UHFFFAOYSA-N
Formula: C16H15NO5
SMILES: CC(C)Oc1ccccc1OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 301.29

Physical Properties

Property code	Value	Unit	Source
gf	-16.41	kJ/mol	Joback Method
hf	-316.51	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	84.86	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	3.601		Crippen Method
mcvol	219.510	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	878.91	K	Joback Method
tc	1131.32	K	Joback Method
tf	570.96	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.47	J/mol×K	878.91	Joback Method
cpg	655.52	J/mol×K	920.98	Joback Method
cpg	666.19	J/mol×K	963.05	Joback Method
cpg	675.50	J/mol×K	1005.12	Joback Method
cpg	683.50	J/mol×K	1047.19	Joback Method
cpg	690.22	J/mol×K	1089.25	Joback Method
cpg	695.70	J/mol×K	1131.32	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/cbook.cgi?ID=U299036&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume