4-Cyanobenzoic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C17H15NO3/c1-12(2)20-15-5-3-4-6-16(15)21-17(19)14-9-7-13(11-18)8-10-14/h
InchiKey: SJIOOBQMRVGMGT-UHFFFAOYSA-N
Formula: C17H15NO3
SMILES: CC(C)Oc1ccccc1OC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 281.31

Physical Properties

Property code	Value	Unit	Source
gf	89.64	kJ/mol	Joback Method
hf	-161.51	kJ/mol	Joback Method
hfus	29.05	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.565		Crippen Method
mcvol	217.560	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1996.40		NIST Webbook
tb	852.03	K	Joback Method
tc	1093.45	K	Joback Method
tf	503.61	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.50	J/mol×K	852.03	Joback Method
cpg	629.68	J/mol×K	892.27	Joback Method
cpg	640.63	J/mol×K	932.50	Joback Method
cpg	650.36	J/mol×K	972.74	Joback Method
cpg	658.91	J/mol×K	1012.98	Joback Method
cpg	666.30	J/mol×K	1053.22	Joback Method
cpg	672.56	J/mol×K	1093.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292660&Units=SI

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