3-Fluorobenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C14H8FNO2/c15-12-3-1-2-11(8-12)14(17)18-13-6-4-10(9-16)5-7-13/h1-8H
InchiKey: NHVRPBNIRMXORF-UHFFFAOYSA-N
Formula: C14H8FNO2
SMILES: N#Cc1ccc(OC(=O)c2cccc(F)c2)cc1
Mol. weight [g/mol]: 241.22

Physical Properties

Property code	Value	Unit	Source
gf	-22.99	kJ/mol	Joback Method
hf	-158.20	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	2.917		Crippen Method
mcvol	171.190	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1905.00		NIST Webbook
tb	760.68	K	Joback Method
tc	1004.63	K	Joback Method
tf	463.16	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.52	J/mol×K	760.68	Joback Method
cpg	450.33	J/mol×K	801.34	Joback Method
cpg	460.14	J/mol×K	842.00	Joback Method
cpg	469.00	J/mol×K	882.66	Joback Method
cpg	476.94	J/mol×K	923.31	Joback Method
cpg	484.00	J/mol×K	963.97	Joback Method
cpg	490.21	J/mol×K	1004.63	Joback Method

Sources

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=U307728&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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