3-Fluoro-4-trifluoromethylbenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C15H7F4NO2/c16-13-7-10(3-6-12(13)15(17,18)19)14(21)22-11-4-1-9(8-20)2-5

InchiKey: VYNHUXCJIDEODH-UHFFFAOYSA-N

Formula: C15H7F4NO2

SMILES: N#Cc1ccc(OC(=O)c2ccc(C(F)(F)F)c(F)c2)cc1

Mol. weight [g/mol]: 309.22

Physical Properties

Property code	Value	Unit	Source
gf	-605.79	kJ/mol	Joback Method
hf	-787.39	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.935		Crippen Method
mcvol	190.590	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1983.00		NIST Webbook
rinpol	1983.00		NIST Webbook
tb	783.12	K	Joback Method
tc	1007.15	K	Joback Method
tf	491.14	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.42	J/mol×K	783.12	Joback Method
cpg	525.19	J/mol×K	820.46	Joback Method
cpg	534.08	J/mol×K	857.80	Joback Method
cpg	542.14	J/mol×K	895.13	Joback Method
cpg	549.42	J/mol×K	932.47	Joback Method
cpg	555.97	J/mol×K	969.81	Joback Method
cpg	561.84	J/mol×K	1007.15	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=U357945&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

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