2,4,5-Trifluoro-3-methoxybenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C15H8F3NO3/c1-21-14-12(17)10(6-11(16)13(14)18)15(20)22-9-4-2-8(7-19)3-5

InchiKey: GCPIQTCGKUSQHB-UHFFFAOYSA-N

Formula: C15H8F3NO3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2ccc(C#N)cc2)c1F

Mol. weight [g/mol]: 307.22

Physical Properties

Property code	Value	Unit	Source
gf	-538.08	kJ/mol	Joback Method
hf	-737.69	kJ/mol	Joback Method
hfus	35.46	kJ/mol	Joback Method
hvap	76.44	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.203		Crippen Method
mcvol	194.690	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	2225.00		NIST Webbook
tb	819.46	K	Joback Method
tc	1041.32	K	Joback Method
tf	535.40	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.12	J/mol×K	819.46	Joback Method
cpg	535.79	J/mol×K	856.44	Joback Method
cpg	544.55	J/mol×K	893.41	Joback Method
cpg	552.39	J/mol×K	930.39	Joback Method
cpg	559.31	J/mol×K	967.36	Joback Method
cpg	565.31	J/mol×K	1004.34	Joback Method
cpg	570.37	J/mol×K	1041.32	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=U357618&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