2,3,4-Trifluorobenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C14H6F3NO2/c15-11-6-5-10(12(16)13(11)17)14(19)20-9-3-1-8(7-18)2-4-9/h1-
InchiKey: YGRHCLPAJIHTDB-UHFFFAOYSA-N
Formula: C14H6F3NO2
SMILES: N#Cc1ccc(OC(=O)c2ccc(F)c(F)c2F)cc1
Mol. weight [g/mol]: 277.20

Physical Properties

Property code	Value	Unit	Source
gf	-431.87	kJ/mol	Joback Method
hf	-573.36	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	71.14	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.195		Crippen Method
mcvol	174.730	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	769.18	K	Joback Method
tc	995.33	K	Joback Method
tf	489.38	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.62	J/mol×K	769.18	Joback Method
cpg	461.19	J/mol×K	806.87	Joback Method
cpg	469.93	J/mol×K	844.56	Joback Method
cpg	477.86	J/mol×K	882.25	Joback Method
cpg	484.99	J/mol×K	919.95	Joback Method
cpg	491.35	J/mol×K	957.64	Joback Method
cpg	496.96	J/mol×K	995.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308034&Units=SI
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

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