3-Trifluoromethylbenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C15H8F3NO2/c16-15(17,18)12-3-1-2-11(8-12)14(20)21-13-6-4-10(9-19)5-7-13

InchiKey: QMHXNDKFGOVRPY-UHFFFAOYSA-N

Formula: C15H8F3NO2

SMILES: N#Cc1ccc(OC(=O)c2cccc(C(F)(F)F)c2)cc1

Mol. weight [g/mol]: 291.22

Physical Properties

Property code	Value	Unit	Source
gf	-401.35	kJ/mol	Joback Method
hf	-579.81	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	70.75	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.796		Crippen Method
mcvol	188.820	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1896.00		NIST Webbook
tb	778.87	K	Joback Method
tc	1010.93	K	Joback Method
tf	478.03	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.41	J/mol×K	778.87	Joback Method
cpg	519.77	J/mol×K	817.55	Joback Method
cpg	529.17	J/mol×K	856.22	Joback Method
cpg	537.66	J/mol×K	894.90	Joback Method
cpg	545.33	J/mol×K	933.57	Joback Method
cpg	552.23	J/mol×K	972.25	Joback Method
cpg	558.42	J/mol×K	1010.93	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=U307680&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