4-Fluoro-2-trifluoromethylbenzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H10F4O2/c1-9-3-2-4-11(7-9)21-14(20)12-6-5-10(16)8-13(12)15(17,18)19/h

InchiKey: LRENRDQFLLRAHX-UHFFFAOYSA-N

Formula: C15H10F4O2

SMILES: Cc1cccc(OC(=O)c2ccc(F)cc2C(F)(F)F)c1

Mol. weight [g/mol]: 298.23

Physical Properties

Property code	Value	Unit	Source
gf	-738.97	kJ/mol	Joback Method
hf	-952.27	kJ/mol	Joback Method
hfus	29.21	kJ/mol	Joback Method
hvap	60.11	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.372		Crippen Method
mcvol	189.210	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	681.04	K	Joback Method
tc	893.48	K	Joback Method
tf	426.15	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.78	J/mol×K	681.04	Joback Method
cpg	511.73	J/mol×K	716.45	Joback Method
cpg	523.70	J/mol×K	751.85	Joback Method
cpg	534.75	J/mol×K	787.26	Joback Method
cpg	544.92	J/mol×K	822.66	Joback Method
cpg	554.26	J/mol×K	858.07	Joback Method
cpg	562.82	J/mol×K	893.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357664&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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