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

Inchi: InChI=1S/C15H10F4O3/c1-21-10-3-5-11(6-4-10)22-14(20)9-2-7-12(13(16)8-9)15(17,18)1

InchiKey: WCLMIGFNWHGQER-UHFFFAOYSA-N

Formula: C15H10F4O3

SMILES: COc1ccc(OC(=O)c2ccc(C(F)(F)F)c(F)c2)cc1

Mol. weight [g/mol]: 314.23

Physical Properties

Property code	Value	Unit	Source
gf	-843.97	kJ/mol	Joback Method
hf	-1084.49	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.072		Crippen Method
mcvol	195.080	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1895.00		NIST Webbook
tb	703.46	K	Joback Method
tc	913.82	K	Joback Method
tf	448.38	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.99	J/mol×K	703.46	Joback Method
cpg	536.60	J/mol×K	738.52	Joback Method
cpg	548.25	J/mol×K	773.58	Joback Method
cpg	558.99	J/mol×K	808.64	Joback Method
cpg	568.85	J/mol×K	843.70	Joback Method
cpg	577.85	J/mol×K	878.76	Joback Method
cpg	586.02	J/mol×K	913.82	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=U357943&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