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

Inchi: InChI=1S/C14H7F5O3/c1-21-13-11(18)9(5-10(17)12(13)19)14(20)22-8-3-6(15)2-7(16)4-8

InchiKey: ZKHDHVKIKPMOFG-UHFFFAOYSA-N

Formula: C14H7F5O3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2cc(F)cc(F)c2)c1F

Mol. weight [g/mol]: 318.20

Physical Properties

Property code	Value	Unit	Source
gf	-1078.93	kJ/mol	Joback Method
hf	-1285.62	kJ/mol	Joback Method
hfus	37.14	kJ/mol	Joback Method
hvap	62.76	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.610		Crippen Method
mcvol	182.760	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1749.00		NIST Webbook
tb	698.02	K	Joback Method
tc	895.90	K	Joback Method
tf	472.84	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.05	J/mol×K	698.02	Joback Method
cpg	484.93	J/mol×K	731.00	Joback Method
cpg	495.14	J/mol×K	763.98	Joback Method
cpg	504.66	J/mol×K	796.96	Joback Method
cpg	513.49	J/mol×K	829.94	Joback Method
cpg	521.61	J/mol×K	862.92	Joback Method
cpg	529.02	J/mol×K	895.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357609&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