2-Fluoro-3-trifluoromethylbenzoic acid, 3,5-difluophenyl ester

Inchi: InChI=1S/C14H6F6O2/c15-7-4-8(16)6-9(5-7)22-13(21)10-2-1-3-11(12(10)17)14(18,19)20

InchiKey: XXABOBBXNZSSHT-UHFFFAOYSA-N

Formula: C14H6F6O2

SMILES: O=C(Oc1cc(F)cc(F)c1)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 320.19

Physical Properties

Property code	Value	Unit	Source
gf	-1146.64	kJ/mol	Joback Method
hf	-1335.32	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	56.92	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.342		Crippen Method
mcvol	178.660	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	661.68	K	Joback Method
tc	860.81	K	Joback Method
tf	428.58	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.43	J/mol×K	661.68	Joback Method
cpg	474.59	J/mol×K	694.87	Joback Method
cpg	484.94	J/mol×K	728.06	Joback Method
cpg	494.52	J/mol×K	761.25	Joback Method
cpg	503.37	J/mol×K	794.43	Joback Method
cpg	511.52	J/mol×K	827.62	Joback Method
cpg	519.00	J/mol×K	860.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357641&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