6-Fluoro-3-trifluoromethylbenzoic acid, 2,3-dichlorophenyl ester

Other names: 6-Fluoro-3-trifluorobenzoic acid, 2,3-dichlorophenyl ester
Inchi: InChI=1S/C14H6Cl2F4O2/c15-9-2-1-3-11(12(9)16)22-13(21)8-6-7(14(18,19)20)4-5-10(8)
InchiKey: WPODOPQVUWUHAY-UHFFFAOYSA-N
Formula: C14H6Cl2F4O2
SMILES: O=C(Oc1cccc(Cl)c1Cl)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 353.10

Physical Properties

Property code	Value	Unit	Source
gf	-780.88	kJ/mol	Joback Method
hf	-974.58	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	67.32	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.370		Crippen Method
mcvol	199.600	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
tb	738.00	K	Joback Method
tc	960.76	K	Joback Method
tf	487.24	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.48	J/mol×K	738.00	Joback Method
cpg	502.52	J/mol×K	775.13	Joback Method
cpg	511.67	J/mol×K	812.25	Joback Method
cpg	520.00	J/mol×K	849.38	Joback Method
cpg	527.53	J/mol×K	886.51	Joback Method
cpg	534.33	J/mol×K	923.63	Joback Method
cpg	540.44	J/mol×K	960.76	Joback Method

Sources

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=U343789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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