Isophthalic acid, monochloride, 3-fluorophenyl ester

Inchi: InChI=1S/C14H8ClFO3/c15-13(17)9-3-1-4-10(7-9)14(18)19-12-6-2-5-11(16)8-12/h1-8H

InchiKey: UOLGUVXLXFDAMO-UHFFFAOYSA-N

Formula: C14H8ClFO3

SMILES: O=C(Cl)c1cccc(C(=O)Oc2cccc(F)c2)c1

Mol. weight [g/mol]: 278.66

Physical Properties

Property code	Value	Unit	Source
gf	-297.02	kJ/mol	Joback Method
hf	-451.40	kJ/mol	Joback Method
hfus	30.98	kJ/mol	Joback Method
hvap	72.10	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.424		Crippen Method
mcvol	183.620	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	749.90	K	Joback Method
tc	991.10	K	Joback Method
tf	478.02	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.98	J/mol×K	749.90	Joback Method
cpg	468.13	J/mol×K	790.10	Joback Method
cpg	478.24	J/mol×K	830.30	Joback Method
cpg	487.35	J/mol×K	870.50	Joback Method
cpg	495.50	J/mol×K	910.70	Joback Method
cpg	502.72	J/mol×K	950.90	Joback Method
cpg	509.06	J/mol×K	991.10	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=U344675&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