Succinic acid, 2-chloro-6-fluorophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C16H11ClF2O4/c17-12-5-2-6-13(19)16(12)23-15(21)8-7-14(20)22-11-4-1-3-10

InchiKey: FMPDHZKQSWCNQJ-UHFFFAOYSA-N

Formula: C16H11ClF2O4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)Oc1cccc(F)c1

Mol. weight [g/mol]: 340.71

Physical Properties

Property code	Value	Unit	Source
gf	-589.62	kJ/mol	Joback Method
hf	-832.48	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	78.81	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.909		Crippen Method
mcvol	219.440	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	822.33	K	Joback Method
tc	1045.29	K	Joback Method
tf	535.90	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.20	J/mol×K	822.33	Joback Method
cpg	604.11	J/mol×K	859.49	Joback Method
cpg	613.98	J/mol×K	896.65	Joback Method
cpg	622.82	J/mol×K	933.81	Joback Method
cpg	630.64	J/mol×K	970.97	Joback Method
cpg	637.47	J/mol×K	1008.13	Joback Method
cpg	643.31	J/mol×K	1045.29	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=U390333&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