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

Inchi: InChI=1S/C19H18ClFO4/c1-2-6-13-7-3-4-10-16(13)24-17(22)11-12-18(23)25-19-14(20)8

InchiKey: ZTRWBWLJSQKBGL-UHFFFAOYSA-N

Formula: C19H18ClFO4

SMILES: CCCc1ccccc1OC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 364.80

Physical Properties

Property code	Value	Unit	Source
gf	-369.55	kJ/mol	Joback Method
hf	-698.29	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	86.31	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.723		Crippen Method
mcvol	259.940	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	891.70	K	Joback Method
tc	1115.74	K	Joback Method
tf	569.12	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.15	J/mol×K	891.70	Joback Method
cpg	764.19	J/mol×K	929.04	Joback Method
cpg	775.02	J/mol×K	966.38	Joback Method
cpg	784.67	J/mol×K	1003.72	Joback Method
cpg	793.18	J/mol×K	1041.06	Joback Method
cpg	800.55	J/mol×K	1078.40	Joback Method
cpg	806.82	J/mol×K	1115.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390393&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

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