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

Inchi: InChI=1S/C15H18ClFO4/c1-3-10(4-2)20-13(18)8-9-14(19)21-15-11(16)6-5-7-12(15)17/h5

InchiKey: OKPQAHSMSGVVDX-UHFFFAOYSA-N

Formula: C15H18ClFO4

SMILES: CCC(CC)OC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 316.75

Physical Properties

Property code	Value	Unit	Source
gf	-508.45	kJ/mol	Joback Method
hf	-846.07	kJ/mol	Joback Method
hfus	37.20	kJ/mol	Joback Method
hvap	74.08	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.896		Crippen Method
mcvol	227.340	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	768.08	K	Joback Method
tc	972.20	K	Joback Method
tf	470.10	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.25	J/mol×K	768.08	Joback Method
cpg	640.50	J/mol×K	802.10	Joback Method
cpg	652.83	J/mol×K	836.12	Joback Method
cpg	664.24	J/mol×K	870.14	Joback Method
cpg	674.75	J/mol×K	904.16	Joback Method
cpg	684.35	J/mol×K	938.18	Joback Method
cpg	693.05	J/mol×K	972.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370918&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