Succinic acid, 2-chloro-6-fluorophenyl dec-4-en-1-yl ester

Inchi: InChI=1S/C20H26ClFO4/c1-2-3-4-5-6-7-8-9-15-25-18(23)13-14-19(24)26-20-16(21)11-10

InchiKey: ZSHKOIKIUWTGDK-VOTSOKGWSA-N

Formula: C20H26ClFO4

SMILES: CCCCCC=CCCCOC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 384.87

Physical Properties

Property code	Value	Unit	Source
gf	-383.69	kJ/mol	Joback Method
hf	-826.77	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.625		Crippen Method
mcvol	293.490	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2592.00		NIST Webbook
rinpol	2592.00		NIST Webbook
tb	887.08	K	Joback Method
tc	1093.33	K	Joback Method
tf	536.37	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.90	J/mol×K	887.08	Joback Method
cpg	898.00	J/mol×K	921.45	Joback Method
cpg	911.06	J/mol×K	955.83	Joback Method
cpg	923.09	J/mol×K	990.20	Joback Method
cpg	934.14	J/mol×K	1024.58	Joback Method
cpg	944.24	J/mol×K	1058.95	Joback Method
cpg	953.43	J/mol×K	1093.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391177&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

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