Succinic acid, 2-chloro-6-fluorobenzyl undecyl ester

Inchi: InChI=1S/C22H32ClFO4/c1-2-3-4-5-6-7-8-9-10-16-27-21(25)14-15-22(26)28-17-18-19(23

InchiKey: MMQLMDCSNOBZOR-UHFFFAOYSA-N

Formula: C22H32ClFO4

SMILES: CCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1Cl

Mol. weight [g/mol]: 414.94

Physical Properties

Property code	Value	Unit	Source
gf	-447.07	kJ/mol	Joback Method
hf	-985.27	kJ/mol	Joback Method
hfus	58.85	kJ/mol	Joback Method
hvap	90.05	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.377		Crippen Method
mcvol	325.970	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	928.68	K	Joback Method
tc	1137.77	K	Joback Method
tf	563.99	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.61	J/mol×K	928.68	Joback Method
cpg	1045.68	J/mol×K	963.53	Joback Method
cpg	1059.49	J/mol×K	998.38	Joback Method
cpg	1072.06	J/mol×K	1033.22	Joback Method
cpg	1083.43	J/mol×K	1068.07	Joback Method
cpg	1093.62	J/mol×K	1102.92	Joback Method
cpg	1102.66	J/mol×K	1137.77	Joback Method

Sources

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=U380867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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