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

Inchi: InChI=1S/C23H34ClFO4/c1-2-3-4-5-6-7-8-9-10-11-17-28-22(26)15-16-23(27)29-18-19-2

InchiKey: BKTMEZXGELCJAR-UHFFFAOYSA-N

Formula: C23H34ClFO4

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

Mol. weight [g/mol]: 428.96

Physical Properties

Property code	Value	Unit	Source
gf	-438.65	kJ/mol	Joback Method
hf	-1005.91	kJ/mol	Joback Method
hfus	61.44	kJ/mol	Joback Method
hvap	92.27	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.767		Crippen Method
mcvol	340.060	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
tb	951.56	K	Joback Method
tc	1165.01	K	Joback Method
tf	575.26	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.13	J/mol×K	951.56	Joback Method
cpg	1106.48	J/mol×K	987.14	Joback Method
cpg	1120.48	J/mol×K	1022.71	Joback Method
cpg	1133.17	J/mol×K	1058.29	Joback Method
cpg	1144.58	J/mol×K	1093.86	Joback Method
cpg	1154.74	J/mol×K	1129.44	Joback Method
cpg	1163.70	J/mol×K	1165.01	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=U380868&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