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

Inchi: InChI=1S/C25H38ClFO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-30-24(28)17-18-25(29)31-20

InchiKey: TYTVXECXYFEKRA-UHFFFAOYSA-N

Formula: C25H38ClFO4

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

Mol. weight [g/mol]: 457.02

Physical Properties

Property code	Value	Unit	Source
gf	-421.81	kJ/mol	Joback Method
hf	-1047.19	kJ/mol	Joback Method
hfus	66.62	kJ/mol	Joback Method
hvap	96.72	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.547		Crippen Method
mcvol	368.240	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	3104.00		NIST Webbook
rinpol	3104.00		NIST Webbook
tb	997.32	K	Joback Method
tc	1222.60	K	Joback Method
tf	597.80	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.69	J/mol×K	997.32	Joback Method
cpg	1229.62	J/mol×K	1034.87	Joback Method
cpg	1244.01	J/mol×K	1072.41	Joback Method
cpg	1256.91	J/mol×K	1109.96	Joback Method
cpg	1268.35	J/mol×K	1147.51	Joback Method
cpg	1278.38	J/mol×K	1185.05	Joback Method
cpg	1287.06	J/mol×K	1222.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380870&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