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

Inchi: InChI=1S/C27H42ClFO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-32-26(30)19-20-27(31

InchiKey: AAKOKJAWTBKOFJ-UHFFFAOYSA-N

Formula: C27H42ClFO4

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

Mol. weight [g/mol]: 485.07

Physical Properties

Property code	Value	Unit	Source
gf	-404.97	kJ/mol	Joback Method
hf	-1088.47	kJ/mol	Joback Method
hfus	71.80	kJ/mol	Joback Method
hvap	101.18	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	8.327		Crippen Method
mcvol	396.420	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinpol	3304.00		NIST Webbook
rinpol	3304.00		NIST Webbook
tb	1043.08	K	Joback Method
tc	1284.84	K	Joback Method
tf	620.34	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.90	J/mol×K	1043.08	Joback Method
cpg	1354.52	J/mol×K	1083.37	Joback Method
cpg	1369.32	J/mol×K	1123.67	Joback Method
cpg	1382.38	J/mol×K	1163.96	Joback Method
cpg	1393.76	J/mol×K	1204.25	Joback Method
cpg	1403.53	J/mol×K	1244.55	Joback Method
cpg	1411.76	J/mol×K	1284.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380872&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