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

Inchi: InChI=1S/C17H22ClFO4/c1-2-3-4-5-11-22-16(20)9-10-17(21)23-12-13-14(18)7-6-8-15(1

InchiKey: JJUGVGLWXXLEAX-UHFFFAOYSA-N

Formula: C17H22ClFO4

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

Mol. weight [g/mol]: 344.81

Physical Properties

Property code	Value	Unit	Source
gf	-489.17	kJ/mol	Joback Method
hf	-882.07	kJ/mol	Joback Method
hfus	45.90	kJ/mol	Joback Method
hvap	78.92	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.426		Crippen Method
mcvol	255.520	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
tb	814.28	K	Joback Method
tc	1014.35	K	Joback Method
tf	507.64	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.88	J/mol×K	814.28	Joback Method
cpg	751.62	J/mol×K	847.62	Joback Method
cpg	764.38	J/mol×K	880.97	Joback Method
cpg	776.17	J/mol×K	914.31	Joback Method
cpg	787.02	J/mol×K	947.66	Joback Method
cpg	796.92	J/mol×K	981.00	Joback Method
cpg	805.90	J/mol×K	1014.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380863&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