Succinic acid, 3,5-difluorophenyl 6-chlorohexyl ester

Inchi: InChI=1S/C16H19ClF2O4/c17-7-3-1-2-4-8-22-15(20)5-6-16(21)23-14-10-12(18)9-13(19)1

InchiKey: FOTKYZDDEIFNKA-UHFFFAOYSA-N

Formula: C16H19ClF2O4

SMILES: O=C(CCC(=O)Oc1cc(F)cc(F)c1)OCCCCCCCl

Mol. weight [g/mol]: 348.77

Physical Properties

Property code	Value	Unit	Source
gf	-692.40	kJ/mol	Joback Method
hf	-1057.54	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	75.87	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.993		Crippen Method
mcvol	243.200	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	790.67	K	Joback Method
tc	985.82	K	Joback Method
tf	496.96	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.40	J/mol×K	790.67	Joback Method
cpg	702.38	J/mol×K	823.19	Joback Method
cpg	714.47	J/mol×K	855.72	Joback Method
cpg	725.68	J/mol×K	888.24	Joback Method
cpg	736.02	J/mol×K	920.77	Joback Method
cpg	745.50	J/mol×K	953.29	Joback Method
cpg	754.13	J/mol×K	985.82	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=U358036&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