Succinic acid, 2-chloro-6-fluorophenyl 3-heptyl ester

Inchi: InChI=1S/C17H22ClFO4/c1-3-5-7-12(4-2)22-15(20)10-11-16(21)23-17-13(18)8-6-9-14(1
InchiKey: BKVDMNWMAQAXTI-UHFFFAOYSA-N
Formula: C17H22ClFO4
SMILES: CCCCC(CC)OC(=O)CCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 344.81

Physical Properties

Property code	Value	Unit	Source
gf	-491.61	kJ/mol	Joback Method
hf	-887.35	kJ/mol	Joback Method
hfus	42.38	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.677		Crippen Method
mcvol	255.520	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	813.84	K	Joback Method
tc	1016.05	K	Joback Method
tf	492.64	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.44	J/mol×K	813.84	Joback Method
cpg	752.32	J/mol×K	847.54	Joback Method
cpg	765.19	J/mol×K	881.24	Joback Method
cpg	777.06	J/mol×K	914.95	Joback Method
cpg	787.95	J/mol×K	948.65	Joback Method
cpg	797.87	J/mol×K	982.35	Joback Method
cpg	806.84	J/mol×K	1016.05	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U390604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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