Succinic acid, 2-chloro-6-fluorophenyl hex-5-en-1-yl ester

Inchi: InChI=1S/C16H18ClFO4/c1-2-3-4-5-11-21-14(19)9-10-15(20)22-16-12(17)7-6-8-13(16)18

InchiKey: ITIREZLSGRNLPR-UHFFFAOYSA-N

Formula: C16H18ClFO4

SMILES: C=CCCCCOC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 328.76

Physical Properties

Property code	Value	Unit	Source
gf	-409.75	kJ/mol	Joback Method
hf	-736.00	kJ/mol	Joback Method
hfus	42.03	kJ/mol	Joback Method
hvap	76.02	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.064		Crippen Method
mcvol	237.130	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	788.08	K	Joback Method
tc	990.76	K	Joback Method
tf	494.61	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.92	J/mol×K	788.08	Joback Method
cpg	668.81	J/mol×K	821.86	Joback Method
cpg	680.78	J/mol×K	855.64	Joback Method
cpg	691.86	J/mol×K	889.42	Joback Method
cpg	702.06	J/mol×K	923.20	Joback Method
cpg	711.39	J/mol×K	956.98	Joback Method
cpg	719.87	J/mol×K	990.76	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391286&Units=SI

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