Succinic acid, 2-chloro-6-fluorophenyl trans-hex-3-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: GWXMBNAANSITOC-ONEGZZNKSA-N

Formula: C16H18ClFO4

SMILES: CCC=CCCOC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 328.76

Physical Properties

Property code	Value	Unit	Source
gf	-417.37	kJ/mol	Joback Method
hf	-744.21	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.064		Crippen Method
mcvol	237.130	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	795.56	K	Joback Method
tc	1001.35	K	Joback Method
tf	491.29	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.06	J/mol×K	795.56	Joback Method
cpg	668.95	J/mol×K	829.86	Joback Method
cpg	680.93	J/mol×K	864.16	Joback Method
cpg	692.04	J/mol×K	898.46	Joback Method
cpg	702.29	J/mol×K	932.75	Joback Method
cpg	711.70	J/mol×K	967.05	Joback Method
cpg	720.30	J/mol×K	1001.35	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=U391118&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