Succinic acid, 3-chlorophenyl 2-fluoroethyl ester

Inchi: InChI=1S/C12H12ClFO4/c13-9-2-1-3-10(8-9)18-12(16)5-4-11(15)17-7-6-14/h1-3,8H,4-7H

InchiKey: LJEYTRNHKVESAT-UHFFFAOYSA-N

Formula: C12H12ClFO4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCCF

Mol. weight [g/mol]: 274.67

Physical Properties

Property code	Value	Unit	Source
gf	-521.64	kJ/mol	Joback Method
hf	-767.40	kJ/mol	Joback Method
hfus	33.34	kJ/mol	Joback Method
hvap	67.12	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.538		Crippen Method
mcvol	185.070	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1983.00		NIST Webbook
rinpol	1983.00		NIST Webbook
tb	694.90	K	Joback Method
tc	901.44	K	Joback Method
tf	438.77	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.38	J/mol×K	694.90	Joback Method
cpg	481.18	J/mol×K	729.32	Joback Method
cpg	492.21	J/mol×K	763.75	Joback Method
cpg	502.46	J/mol×K	798.17	Joback Method
cpg	511.94	J/mol×K	832.59	Joback Method
cpg	520.66	J/mol×K	867.01	Joback Method
cpg	528.62	J/mol×K	901.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390883&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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