Succinic acid, 2-chloro-6-fluorophenyl 2-methoxyethyl ester

Inchi: InChI=1S/C13H14ClFO5/c1-18-7-8-19-11(16)5-6-12(17)20-13-9(14)3-2-4-10(13)15/h2-4
InchiKey: KEWGRLXVORPENA-UHFFFAOYSA-N
Formula: C13H14ClFO5
SMILES: COCCOC(=O)CCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 304.70

Physical Properties

Property code	Value	Unit	Source
gf	-627.85	kJ/mol	Joback Method
hf	-931.73	kJ/mol	Joback Method
hfus	36.73	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.354		Crippen Method
mcvol	205.030	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	745.18	K	Joback Method
tc	948.83	K	Joback Method
tf	484.79	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.22	J/mol×K	745.18	Joback Method
cpg	557.20	J/mol×K	779.12	Joback Method
cpg	568.33	J/mol×K	813.06	Joback Method
cpg	578.63	J/mol×K	847.00	Joback Method
cpg	588.08	J/mol×K	880.94	Joback Method
cpg	596.65	J/mol×K	914.88	Joback Method
cpg	604.36	J/mol×K	948.83	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=U390743&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