Succinic acid, 2,3-dichlorophenyl 2-fluoroethyl ester

Inchi: InChI=1S/C12H11Cl2FO4/c13-8-2-1-3-9(12(8)14)19-11(17)5-4-10(16)18-7-6-15/h1-3H,4-

InchiKey: JEMZDMMXWQFTOK-UHFFFAOYSA-N

Formula: C12H11Cl2FO4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)OCCF

Mol. weight [g/mol]: 309.12

Physical Properties

Property code	Value	Unit	Source
gf	-543.20	kJ/mol	Joback Method
hf	-794.61	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	72.17	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.192		Crippen Method
mcvol	197.310	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	737.31	K	Joback Method
tc	948.04	K	Joback Method
tf	481.21	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.13	J/mol×K	737.31	Joback Method
cpg	501.85	J/mol×K	772.43	Joback Method
cpg	511.80	J/mol×K	807.55	Joback Method
cpg	520.96	J/mol×K	842.67	Joback Method
cpg	529.35	J/mol×K	877.80	Joback Method
cpg	536.95	J/mol×K	912.92	Joback Method
cpg	543.78	J/mol×K	948.04	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=U390885&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