Succinic acid, 2,2-dichloroethyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C13H13Cl2FO5/c1-19-10-6-8(16)2-3-9(10)21-13(18)5-4-12(17)20-7-11(14)15/h

InchiKey: GJNUDBKKMAASDY-UHFFFAOYSA-N

Formula: C13H13Cl2FO5

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 339.15

Physical Properties

Property code	Value	Unit	Source
hfus	40.57	kJ/mol	Joback Method
logp	2.867		Crippen Method
mcvol	217.270	ml/mol	McGowan Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	611.70	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	9.22730e+01
Coeff. B	8.99420e-01
Coeff. C	-3.40720e-04
Coeff. D	-2.67000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390901&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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