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

Inchi: InChI=1S/C12H11ClF2O4/c13-8-2-1-3-9(15)12(8)19-11(17)5-4-10(16)18-7-6-14/h1-3H,4-

InchiKey: BMSCQCSFYNMALN-UHFFFAOYSA-N

Formula: C12H11ClF2O4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)OCCF

Mol. weight [g/mol]: 292.66

Physical Properties

Property code	Value	Unit	Source
gf	-726.08	kJ/mol	Joback Method
hf	-974.98	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	66.97	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.677		Crippen Method
mcvol	186.840	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1915.00		NIST Webbook
tb	699.15	K	Joback Method
tc	898.70	K	Joback Method
tf	451.88	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.08	J/mol×K	699.15	Joback Method
cpg	487.24	J/mol×K	732.41	Joback Method
cpg	497.69	J/mol×K	765.67	Joback Method
cpg	507.44	J/mol×K	798.92	Joback Method
cpg	516.48	J/mol×K	832.18	Joback Method
cpg	524.80	J/mol×K	865.44	Joback Method
cpg	532.42	J/mol×K	898.70	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=U390882&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