Succinic acid, 2-chloro-6-fluorophenyl (2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C17H19Cl2FO4/c18-12-5-2-1-4-11(12)10-23-15(21)8-9-16(22)24-17-13(19)6-3

InchiKey: CZEWUCKWRRZPHB-UHFFFAOYSA-N

Formula: C17H19Cl2FO4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)OCC1CCCCC1Cl

Mol. weight [g/mol]: 377.24

Physical Properties

Property code	Value	Unit	Source
gf	-484.36	kJ/mol	Joback Method
hf	-863.83	kJ/mol	Joback Method
hfus	43.00	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.505		Crippen Method
mcvol	256.900	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	866.59	K	Joback Method
tc	1091.92	K	Joback Method
tf	540.70	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.15	J/mol×K	866.59	Joback Method
cpg	773.77	J/mol×K	904.14	Joback Method
cpg	785.98	J/mol×K	941.70	Joback Method
cpg	796.78	J/mol×K	979.25	Joback Method
cpg	806.20	J/mol×K	1016.81	Joback Method
cpg	814.24	J/mol×K	1054.36	Joback Method
cpg	820.93	J/mol×K	1091.92	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=U391402&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