Succinic acid, 2-chlorophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C16H12ClFO4/c17-13-6-1-2-7-14(13)22-16(20)9-8-15(19)21-12-5-3-4-11(18)10

InchiKey: UIKIOBKKIHUNBZ-UHFFFAOYSA-N

Formula: C16H12ClFO4

SMILES: O=C(CCC(=O)Oc1ccccc1Cl)Oc1cccc(F)c1

Mol. weight [g/mol]: 322.71

Physical Properties

Property code	Value	Unit	Source
gf	-385.18	kJ/mol	Joback Method
hf	-624.90	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.770		Crippen Method
mcvol	217.670	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	818.08	K	Joback Method
tc	1048.23	K	Joback Method
tf	522.79	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.19	J/mol×K	818.08	Joback Method
cpg	598.70	J/mol×K	856.44	Joback Method
cpg	609.08	J/mol×K	894.80	Joback Method
cpg	618.38	J/mol×K	933.15	Joback Method
cpg	626.60	J/mol×K	971.51	Joback Method
cpg	633.78	J/mol×K	1009.87	Joback Method
cpg	639.93	J/mol×K	1048.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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