

Succinic acid, 2-fluorophenyl 4-chloro-2-methylphenyl ester

Inchi:	InChI=1S/C17H14ClFO4/c1-11-10-12(18)6-7-14(11)22-16(20)8-9-17(21)23-15-5-3-2-4-1
InchiKey:	KWRWERQIADSMGB-UHFFFAOYSA-N
Formula:	C17H14ClFO4
SMILES:	Cc1cc(Cl)ccc1OC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]:	336.74

Physical Properties

Property code	Value	Unit	Source
gf	-386.39	kJ/mol	Joback Method
hf	-657.01	kJ/mol	Joback Method
hfus	39.55	kJ/mol	Joback Method
hvap	81.85	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.079		Crippen Method
mvol	231.760	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
tb	845.94	K	Joback Method
tc	1073.89	K	Joback Method
tf	546.58	K	Joback Method
vc	0.886	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.27	J/mol×K	845.94	Joback Method
cpg	651.94	J/mol×K	883.93	Joback Method
cpg	662.46	J/mol×K	921.92	Joback Method
cpg	671.86	J/mol×K	959.91	Joback Method
cpg	680.16	J/mol×K	997.91	Joback Method
cpg	687.36	J/mol×K	1035.90	Joback Method
cpg	693.50	J/mol×K	1073.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U390294&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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