

Succinic acid, 2-chloro-6-fluorophenyl pent-4-en-2-yl ester

Inchi:	InChI=1S/C15H16ClFO4/c1-3-5-10(2)20-13(18)8-9-14(19)21-15-11(16)6-4-7-12(15)17/h
InchiKey:	IIBMPUMKFNXGGJ-UHFFFAOYSA-N
Formula:	C15H16ClFO4
SMILES:	C=CCC(C)OC(=O)CCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	314.74

Physical Properties

Property code	Value	Unit	Source
gf	-420.61	kJ/mol	Joback Method
hf	-720.64	kJ/mol	Joback Method
hfus	35.92	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.672		Crippen Method
mcvol	223.040	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1979.00		NIST Webbook
rinpol	1979.00		NIST Webbook
tb	764.76	K	Joback Method
tc	971.64	K	Joback Method
tf	468.34	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.99	J/molxK	764.76	Joback Method
cpg	614.69	J/molxK	799.24	Joback Method
cpg	626.48	J/molxK	833.72	Joback Method
cpg	637.37	J/molxK	868.20	Joback Method
cpg	647.38	J/molxK	902.68	Joback Method
cpg	656.53	J/molxK	937.16	Joback Method
cpg	664.81	J/molxK	971.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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