

Succinic acid, 2-fluorophenyl hept-1,6-dien-4-yl ester

Inchi:	InChI=1S/C17H19FO4/c1-3-7-13(8-4-2)21-16(19)11-12-17(20)22-15-10-6-5-9-14(15)18/H
InchiKey:	LXAXQLBSFIQXHE-UHFFFAOYSA-N
Formula:	C17H19FO4
SMILES:	<chem>C=CCC(CC=C)OC(=O)CCC(=O)Oc1ccccc1F</chem>
Mol. weight [g/mol]:	306.33

Physical Properties

Property code	Value	Unit	Source
gf	-294.37	kJ/mol	Joback Method
hf	-609.28	kJ/mol	Joback Method
hfus	36.01	kJ/mol	Joback Method
hvap	72.14	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.575		Crippen Method
mvol	234.680	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	764.79	K	Joback Method
tc	966.61	K	Joback Method
tf	446.68	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.54	J/mol×K	764.79	Joback Method
cpg	675.57	J/mol×K	798.43	Joback Method
cpg	688.64	J/mol×K	832.06	Joback Method
cpg	700.78	J/mol×K	865.70	Joback Method
cpg	712.01	J/mol×K	899.34	Joback Method
cpg	722.36	J/mol×K	932.98	Joback Method
cpg	731.84	J/mol×K	966.61	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=U391331&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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