Succinic acid, 2-fluorophenyl 4-octyl ester

Inchi: InChI=1S/C18H25FO4/c1-3-5-9-14(8-4-2)22-17(20)12-13-18(21)23-16-11-7-6-10-15(16)1
InchiKey: SWBXTOCAUFJJPT-UHFFFAOYSA-N
Formula: C18H25FO4
SMILES: CCCCC(CCC)OC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 324.39

Physical Properties

Property code	Value	Unit	Source
gf	-461.63	kJ/mol	Joback Method
hf	-880.78	kJ/mol	Joback Method
hfus	41.16	kJ/mol	Joback Method
hvap	75.71	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.413		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2115.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	794.31	K	Joback Method
tc	990.96	K	Joback Method
tf	461.47	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.34	J/mol×K	794.31	Joback Method
cpg	784.69	J/mol×K	827.09	Joback Method
cpg	799.01	J/mol×K	859.86	Joback Method
cpg	812.32	J/mol×K	892.64	Joback Method
cpg	824.63	J/mol×K	925.41	Joback Method
cpg	835.97	J/mol×K	958.19	Joback Method
cpg	846.35	J/mol×K	990.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389561&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

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