Succinic acid, 2-fluorophenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C18H25FO4/c1-13(11-18(2,3)4)12-22-16(20)9-10-17(21)23-15-8-6-5-7-14(15)1

InchiKey: JSNMPZHITXAJKE-UHFFFAOYSA-N

Formula: C18H25FO4

SMILES: CC(COC(=O)CCC(=O)Oc1ccccc1F)CC(C)(C)C

Mol. weight [g/mol]: 324.39

Physical Properties

Property code	Value	Unit	Source
gf	-458.79	kJ/mol	Joback Method
hf	-889.53	kJ/mol	Joback Method
hfus	33.74	kJ/mol	Joback Method
hvap	74.41	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.127		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	791.08	K	Joback Method
tc	994.20	K	Joback Method
tf	463.89	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.92	J/mol×K	791.08	Joback Method
cpg	786.50	J/mol×K	824.93	Joback Method
cpg	800.99	J/mol×K	858.79	Joback Method
cpg	814.42	J/mol×K	892.64	Joback Method
cpg	826.85	J/mol×K	926.49	Joback Method
cpg	838.30	J/mol×K	960.35	Joback Method
cpg	848.81	J/mol×K	994.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389543&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