Succinic acid, 1-(2-fluorophenyl)ethyl heptyl ester

Inchi: InChI=1S/C19H27FO4/c1-3-4-5-6-9-14-23-18(21)12-13-19(22)24-15(2)16-10-7-8-11-17(1

InchiKey: SDXBCSZHGZUTRK-UHFFFAOYSA-N

Formula: C19H27FO4

SMILES: CCCCCCCOC(=O)CCC(=O)OC(C)c1ccccc1F

Mol. weight [g/mol]: 338.41

Physical Properties

Property code	Value	Unit	Source
gf	-453.21	kJ/mol	Joback Method
hf	-901.42	kJ/mol	Joback Method
hfus	43.75	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.724		Crippen Method
mcvol	271.460	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	817.19	K	Joback Method
tc	1014.05	K	Joback Method
tf	472.74	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.05	J/mol×K	817.19	Joback Method
cpg	842.65	J/mol×K	850.00	Joback Method
cpg	857.18	J/mol×K	882.81	Joback Method
cpg	870.66	J/mol×K	915.62	Joback Method
cpg	883.11	J/mol×K	948.43	Joback Method
cpg	894.55	J/mol×K	981.24	Joback Method
cpg	904.99	J/mol×K	1014.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381396&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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