Succinic acid, 1-(2,6-difluorophenyl)ethyl pentyl ester

Inchi: InChI=1S/C17H22F2O4/c1-3-4-5-11-22-15(20)9-10-16(21)23-12(2)17-13(18)7-6-8-14(17

InchiKey: SJQYZBKFDWTYPU-UHFFFAOYSA-N

Formula: C17H22F2O4

SMILES: CCCCCOC(=O)CCC(=O)OC(C)c1c(F)cccc1F

Mol. weight [g/mol]: 328.35

Physical Properties

Property code	Value	Unit	Source
gf	-674.49	kJ/mol	Joback Method
hf	-1067.72	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.083		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	775.68	K	Joback Method
tc	968.23	K	Joback Method
tf	463.31	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.39	J/mol×K	775.68	Joback Method
cpg	733.89	J/mol×K	807.77	Joback Method
cpg	747.45	J/mol×K	839.86	Joback Method
cpg	760.09	J/mol×K	871.96	Joback Method
cpg	771.81	J/mol×K	904.05	Joback Method
cpg	782.62	J/mol×K	936.14	Joback Method
cpg	792.54	J/mol×K	968.23	Joback Method

Sources

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=U381420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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