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

Inchi: InChI=1S/C16H20F2O4/c1-10(2)9-21-14(19)7-8-15(20)22-11(3)16-12(17)5-4-6-13(16)18

InchiKey: UVEKJCXLQQOMPH-UHFFFAOYSA-N

Formula: C16H20F2O4

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

Mol. weight [g/mol]: 314.32

Physical Properties

Property code	Value	Unit	Source
gf	-685.35	kJ/mol	Joback Method
hf	-1052.36	kJ/mol	Joback Method
hfus	35.15	kJ/mol	Joback Method
hvap	70.71	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.548		Crippen Method
mcvol	230.960	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	752.36	K	Joback Method
tc	947.69	K	Joback Method
tf	437.04	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.18	J/mol×K	752.36	Joback Method
cpg	678.52	J/mol×K	784.92	Joback Method
cpg	691.93	J/mol×K	817.47	Joback Method
cpg	704.44	J/mol×K	850.03	Joback Method
cpg	716.03	J/mol×K	882.58	Joback Method
cpg	726.73	J/mol×K	915.14	Joback Method
cpg	736.53	J/mol×K	947.69	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=U381418&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