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

Inchi: InChI=1S/C20H18F4O4/c1-11(19-13(21)5-3-6-14(19)22)27-17(25)9-10-18(26)28-12(2)20

InchiKey: LDWLFUWBXSCGHV-UHFFFAOYSA-N

Formula: C20H18F4O4

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

Mol. weight [g/mol]: 398.35

Physical Properties

Property code	Value	Unit	Source
gf	-948.14	kJ/mol	Joback Method
hf	-1313.55	kJ/mol	Joback Method
hfus	44.93	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	4.932		Crippen Method
mcvol	267.100	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	879.06	K	Joback Method
tc	1088.16	K	Joback Method
tf	534.76	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.30	J/mol×K	879.06	Joback Method
cpg	820.67	J/mol×K	913.91	Joback Method
cpg	831.89	J/mol×K	948.76	Joback Method
cpg	841.98	J/mol×K	983.61	Joback Method
cpg	850.95	J/mol×K	1018.46	Joback Method
cpg	858.82	J/mol×K	1053.31	Joback Method
cpg	865.62	J/mol×K	1088.16	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=U381430&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