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

Inchi: InChI=1S/C14H16F2O4/c1-3-19-12(17)7-8-13(18)20-9(2)14-10(15)5-4-6-11(14)16/h4-6,9

InchiKey: NSJMCIAAJKEOQK-UHFFFAOYSA-N

Formula: C14H16F2O4

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

Mol. weight [g/mol]: 286.27

Physical Properties

Property code	Value	Unit	Source
gf	-699.75	kJ/mol	Joback Method
hf	-1005.80	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	66.65	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.912		Crippen Method
mcvol	202.780	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
tb	707.04	K	Joback Method
tc	902.16	K	Joback Method
tf	429.50	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.39	J/mol×K	707.04	Joback Method
cpg	568.72	J/mol×K	739.56	Joback Method
cpg	581.25	J/mol×K	772.08	Joback Method
cpg	592.97	J/mol×K	804.60	Joback Method
cpg	603.90	J/mol×K	837.12	Joback Method
cpg	614.03	J/mol×K	869.64	Joback Method
cpg	623.37	J/mol×K	902.16	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=U381416&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