Succinic acid, 3,5-difluorophenyl 2-ethoxyethyl ester

Inchi: InChI=1S/C14H16F2O5/c1-2-19-5-6-20-13(17)3-4-14(18)21-12-8-10(15)7-11(16)9-12/h7
InchiKey: BFVSGCQSXXEKHA-UHFFFAOYSA-N
Formula: C14H16F2O5
SMILES: CCOCCOC(=O)CCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 302.27

Physical Properties

Property code	Value	Unit	Source
gf	-802.31	kJ/mol	Joback Method
hf	-1132.74	kJ/mol	Joback Method
hfus	38.20	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.230		Crippen Method
mcvol	208.650	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1893.00		NIST Webbook
tb	729.90	K	Joback Method
tc	921.70	K	Joback Method
tf	466.73	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.30	J/mol×K	729.90	Joback Method
cpg	594.20	J/mol×K	761.87	Joback Method
cpg	606.29	J/mol×K	793.83	Joback Method
cpg	617.59	J/mol×K	825.80	Joback Method
cpg	628.07	J/mol×K	857.77	Joback Method
cpg	637.73	J/mol×K	889.73	Joback Method
cpg	646.57	J/mol×K	921.70	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=U358032&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