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

Inchi: InChI=1S/C13H14F2O5/c1-18-4-5-19-12(16)2-3-13(17)20-11-7-9(14)6-10(15)8-11/h6-8H

InchiKey: NKLWVJGKVSCJBG-UHFFFAOYSA-N

Formula: C13H14F2O5

SMILES: COCCOC(=O)CCC(=O)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 288.24

Physical Properties

Property code	Value	Unit	Source
gf	-810.73	kJ/mol	Joback Method
hf	-1112.10	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.840		Crippen Method
mcvol	194.560	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	707.02	K	Joback Method
tc	899.99	K	Joback Method
tf	455.46	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.32	J/mol×K	707.02	Joback Method
cpg	540.73	J/mol×K	739.18	Joback Method
cpg	552.40	J/mol×K	771.34	Joback Method
cpg	563.32	J/mol×K	803.51	Joback Method
cpg	573.48	J/mol×K	835.67	Joback Method
cpg	582.86	J/mol×K	867.83	Joback Method
cpg	591.46	J/mol×K	899.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U358031&Units=SI

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