Succinic acid, 3,5-difluorophenyl 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C14H17F2NO4/c1-17(2)5-6-20-13(18)3-4-14(19)21-12-8-10(15)7-11(16)9-12/h

InchiKey: PTUMNWCMFDFKCA-UHFFFAOYSA-N

Formula: C14H17F2NO4

SMILES: CN(C)CCOC(=O)CCC(=O)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 301.29

Physical Properties

Property code	Value	Unit	Source
gf	-586.53	kJ/mol	Joback Method
hf	-932.99	kJ/mol	Joback Method
hfus	40.03	kJ/mol	Joback Method
hvap	69.08	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.755		Crippen Method
mcvol	212.760	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1931.00		NIST Webbook
tb	719.92	K	Joback Method
tc	910.83	K	Joback Method
tf	476.97	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.15	J/mol×K	719.92	Joback Method
cpg	607.48	J/mol×K	751.74	Joback Method
cpg	619.99	J/mol×K	783.56	Joback Method
cpg	631.70	J/mol×K	815.37	Joback Method
cpg	642.61	J/mol×K	847.19	Joback Method
cpg	652.73	J/mol×K	879.01	Joback Method
cpg	662.07	J/mol×K	910.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358033&Units=SI
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

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