Succinic acid, 3,5-difluorophenyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C16H21F2NO4/c1-3-19(4-2)7-8-22-15(20)5-6-16(21)23-14-10-12(17)9-13(18)1

InchiKey: BOFSQWLXIDMAFB-UHFFFAOYSA-N

Formula: C16H21F2NO4

SMILES: CCN(CC)CCOC(=O)CCC(=O)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 329.34

Physical Properties

Property code	Value	Unit	Source
gf	-569.69	kJ/mol	Joback Method
hf	-974.27	kJ/mol	Joback Method
hfus	45.21	kJ/mol	Joback Method
hvap	73.53	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.535		Crippen Method
mcvol	240.940	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
tb	765.68	K	Joback Method
tc	955.60	K	Joback Method
tf	499.51	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.62	J/mol×K	765.68	Joback Method
cpg	717.73	J/mol×K	797.33	Joback Method
cpg	730.94	J/mol×K	828.99	Joback Method
cpg	743.27	J/mol×K	860.64	Joback Method
cpg	754.72	J/mol×K	892.29	Joback Method
cpg	765.32	J/mol×K	923.95	Joback Method
cpg	775.08	J/mol×K	955.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358040&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

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