Succinic acid, 5-fluoro-2-nitrophenyl 3,4-dimethylphenyl ester

Inchi: InChI=1S/C18H16FNO6/c1-11-3-5-14(9-12(11)2)25-17(21)7-8-18(22)26-16-10-13(19)4-6

InchiKey: DIOWEZOGKNUBOZ-UHFFFAOYSA-N

Formula: C18H16FNO6

SMILES: Cc1ccc(OC(=O)CCC(=O)Oc2cc(F)ccc2[N+](=O)[O-])cc1C

Mol. weight [g/mol]: 361.32

Physical Properties

Property code	Value	Unit	Source
gf	-340.12	kJ/mol	Joback Method
hf	-684.14	kJ/mol	Joback Method
hfus	48.92	kJ/mol	Joback Method
hvap	96.95	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	3.642		Crippen Method
mcvol	251.030	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
tb	988.21	K	Joback Method
tc	1230.50	K	Joback Method
tf	684.06	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.28	J/mol×K	988.21	Joback Method
cpg	773.41	J/mol×K	1028.59	Joback Method
cpg	781.15	J/mol×K	1068.97	Joback Method
cpg	787.52	J/mol×K	1109.36	Joback Method
cpg	792.56	J/mol×K	1149.74	Joback Method
cpg	796.27	J/mol×K	1190.12	Joback Method
cpg	798.68	J/mol×K	1230.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357983&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