Succinic acid, 5-fluoro-2-nitrophenyl 2-biphenyl ester

Inchi: InChI=1S/C22H16FNO6/c23-16-10-11-18(24(27)28)20(14-16)30-22(26)13-12-21(25)29-1

InchiKey: DROFBJMREVDMNC-UHFFFAOYSA-N

Formula: C22H16FNO6

SMILES: O=C(CCC(=O)Oc1cc(F)ccc1[N+](=O)[O-])Oc1ccccc1-c1ccccc1

Mol. weight [g/mol]: 409.36

Physical Properties

Property code	Value	Unit	Source
gf	-184.40	kJ/mol	Joback Method
hf	-518.70	kJ/mol	Joback Method
hfus	53.71	kJ/mol	Joback Method
hvap	107.47	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	4.692		Crippen Method
mcvol	283.630	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	3120.00		NIST Webbook
tb	1101.43	K	Joback Method
tc	1363.88	K	Joback Method
tf	743.04	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.46	J/mol×K	1101.43	Joback Method
cpg	886.09	J/mol×K	1145.17	Joback Method
cpg	891.26	J/mol×K	1188.91	Joback Method
cpg	895.03	J/mol×K	1232.66	Joback Method
cpg	897.47	J/mol×K	1276.40	Joback Method
cpg	898.67	J/mol×K	1320.14	Joback Method
cpg	898.69	J/mol×K	1363.88	Joback Method

Sources

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=U357984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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