Sebacic acid, di(3-fluorophenyl) ester

Inchi: InChI=1S/C22H24F2O4/c23-17-9-7-11-19(15-17)27-21(25)13-5-3-1-2-4-6-14-22(26)28-2
InchiKey: QJRKVPXBVFMDCV-UHFFFAOYSA-N
Formula: C22H24F2O4
SMILES: O=C(CCCCCCCCC(=O)Oc1cccc(F)c1)Oc1cccc(F)c1
Mol. weight [g/mol]: 390.42

Physical Properties

Property code	Value	Unit	Source
gf	-517.54	kJ/mol	Joback Method
hf	-929.11	kJ/mol	Joback Method
hfus	51.77	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.597		Crippen Method
mcvol	291.740	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	917.20	K	Joback Method
tc	1131.06	K	Joback Method
tf	561.08	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.03	J/mol×K	917.20	Joback Method
cpg	924.48	J/mol×K	952.84	Joback Method
cpg	936.69	J/mol×K	988.49	Joback Method
cpg	947.70	J/mol×K	1024.13	Joback Method
cpg	957.54	J/mol×K	1059.77	Joback Method
cpg	966.26	J/mol×K	1095.41	Joback Method
cpg	973.88	J/mol×K	1131.06	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=U355022&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