Sebacic acid, 3,5-difluorophenyl isohexyl ester

Inchi: InChI=1S/C22H32F2O4/c1-17(2)10-9-13-27-21(25)11-7-5-3-4-6-8-12-22(26)28-20-15-18
InchiKey: KDAXDNCDYZDKPY-UHFFFAOYSA-N
Formula: C22H32F2O4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 398.48

Physical Properties

Property code	Value	Unit	Source
gf	-632.39	kJ/mol	Joback Method
hf	-1170.92	kJ/mol	Joback Method
hfus	54.21	kJ/mol	Joback Method
hvap	84.46	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.970		Crippen Method
mcvol	315.500	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	890.08	K	Joback Method
tc	1090.97	K	Joback Method
tf	519.66	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.53	J/mol×K	890.08	Joback Method
cpg	1027.50	J/mol×K	923.56	Joback Method
cpg	1042.26	J/mol×K	957.04	Joback Method
cpg	1055.82	J/mol×K	990.52	Joback Method
cpg	1068.21	J/mol×K	1024.00	Joback Method
cpg	1079.45	J/mol×K	1057.49	Joback Method
cpg	1089.58	J/mol×K	1090.97	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=U354527&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