Sebacic acid, 3,5-difluorophenyl hexyl ester

Inchi: InChI=1S/C22H32F2O4/c1-2-3-4-11-14-27-21(25)12-9-7-5-6-8-10-13-22(26)28-20-16-18
InchiKey: FFZUEXJJXVVTIK-UHFFFAOYSA-N
Formula: C22H32F2O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 398.48

Physical Properties

Property code	Value	Unit	Source
gf	-629.95	kJ/mol	Joback Method
hf	-1165.64	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.114		Crippen Method
mcvol	315.500	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2647.00		NIST Webbook
rinpol	2647.00		NIST Webbook
tb	890.52	K	Joback Method
tc	1090.98	K	Joback Method
tf	534.66	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.05	J/mol×K	890.52	Joback Method
cpg	1027.01	J/mol×K	923.93	Joback Method
cpg	1041.77	J/mol×K	957.34	Joback Method
cpg	1055.35	J/mol×K	990.75	Joback Method
cpg	1067.77	J/mol×K	1024.16	Joback Method
cpg	1079.07	J/mol×K	1057.57	Joback Method
cpg	1089.26	J/mol×K	1090.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354528&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

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