Sebacic acid, 3-fluorophenyl hexyl ester

Inchi: InChI=1S/C22H33FO4/c1-2-3-4-11-17-26-21(24)15-9-7-5-6-8-10-16-22(25)27-20-14-12-1
InchiKey: FVYKUIFHBYSLDR-UHFFFAOYSA-N
Formula: C22H33FO4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 380.49

Physical Properties

Property code	Value	Unit	Source
gf	-425.51	kJ/mol	Joback Method
hf	-958.06	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.975		Crippen Method
mcvol	313.730	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	2684.00		NIST Webbook
tb	886.27	K	Joback Method
tc	1087.24	K	Joback Method
tf	521.55	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.47	J/mol×K	886.27	Joback Method
cpg	1020.74	J/mol×K	919.76	Joback Method
cpg	1035.81	J/mol×K	953.26	Joback Method
cpg	1049.70	J/mol×K	986.75	Joback Method
cpg	1062.44	J/mol×K	1020.25	Joback Method
cpg	1074.06	J/mol×K	1053.74	Joback Method
cpg	1084.59	J/mol×K	1087.24	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=U355014&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