Sebacic acid, 1-(2-fluorophenyl)ethyl isobutyl ester

Inchi: InChI=1S/C22H33FO4/c1-17(2)16-26-21(24)14-8-6-4-5-7-9-15-22(25)27-18(3)19-12-10-1

InchiKey: MRLFFIHXGCCGFL-UHFFFAOYSA-N

Formula: C22H33FO4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OC(C)c1ccccc1F

Mol. weight [g/mol]: 380.49

Physical Properties

Property code	Value	Unit	Source
gf	-430.39	kJ/mol	Joback Method
hf	-968.62	kJ/mol	Joback Method
hfus	48.00	kJ/mol	Joback Method
hvap	84.22	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.750		Crippen Method
mcvol	313.730	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	885.39	K	Joback Method
tc	1088.02	K	Joback Method
tf	491.55	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.44	J/mol×K	885.39	Joback Method
cpg	1021.80	J/mol×K	919.16	Joback Method
cpg	1036.91	J/mol×K	952.93	Joback Method
cpg	1050.81	J/mol×K	986.71	Joback Method
cpg	1063.51	J/mol×K	1020.48	Joback Method
cpg	1075.06	J/mol×K	1054.25	Joback Method
cpg	1085.48	J/mol×K	1088.02	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=U380749&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