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

Inchi: InChI=1S/C22H33FO4/c1-18(2)17-27-22(25)14-8-6-4-3-5-7-13-21(24)26-16-15-19-11-9-1

InchiKey: YFYSZUKJFCCQER-UHFFFAOYSA-N

Formula: C22H33FO4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCCc1ccccc1F

Mol. weight [g/mol]: 380.49

Physical Properties

Property code	Value	Unit	Source
gf	-427.95	kJ/mol	Joback Method
hf	-963.34	kJ/mol	Joback Method
hfus	51.52	kJ/mol	Joback Method
hvap	84.61	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.231		Crippen Method
mcvol	313.730	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
tb	885.83	K	Joback Method
tc	1087.56	K	Joback Method
tf	506.55	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.95	J/mol×K	885.83	Joback Method
cpg	1021.27	J/mol×K	919.45	Joback Method
cpg	1036.35	J/mol×K	953.07	Joback Method
cpg	1050.24	J/mol×K	986.69	Joback Method
cpg	1062.96	J/mol×K	1020.32	Joback Method
cpg	1074.54	J/mol×K	1053.94	Joback Method
cpg	1085.01	J/mol×K	1087.56	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=U380744&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