Sebacic acid, 2-fluorophenyl isobutyl ester

Inchi: InChI=1S/C20H29FO4/c1-16(2)15-24-19(22)13-7-5-3-4-6-8-14-20(23)25-18-12-10-9-11-1
InchiKey: DMEVLVNHEHZIOA-UHFFFAOYSA-N
Formula: C20H29FO4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 352.44

Physical Properties

Property code	Value	Unit	Source
gf	-444.79	kJ/mol	Joback Method
hf	-922.06	kJ/mol	Joback Method
hfus	46.34	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.051		Crippen Method
mcvol	285.550	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	840.07	K	Joback Method
tc	1037.81	K	Joback Method
tf	484.01	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.60	J/mol×K	840.07	Joback Method
cpg	901.44	J/mol×K	873.03	Joback Method
cpg	916.17	J/mol×K	905.98	Joback Method
cpg	929.79	J/mol×K	938.94	Joback Method
cpg	942.35	J/mol×K	971.90	Joback Method
cpg	953.86	J/mol×K	1004.86	Joback Method
cpg	964.34	J/mol×K	1037.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354996&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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