Sebacic acid, di(1-(4-fluorophenyl)ethyl) ester

Inchi: InChI=1S/C26H32F2O4/c1-19(21-11-15-23(27)16-12-21)31-25(29)9-7-5-3-4-6-8-10-26(3
InchiKey: RYAOYJQJFNWAPK-UHFFFAOYSA-N
Formula: C26H32F2O4
SMILES: CC(OC(=O)CCCCCCCCC(=O)OC(C)c1ccc(F)cc1)c1ccc(F)cc1
Mol. weight [g/mol]: 446.53

Physical Properties

Property code	Value	Unit	Source
gf	-488.74	kJ/mol	Joback Method
hf	-1022.23	kJ/mol	Joback Method
hfus	55.09	kJ/mol	Joback Method
hvap	95.25	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	6.994		Crippen Method
mcvol	348.100	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2960.00		NIST Webbook
rinpol	2960.00		NIST Webbook
tb	1007.84	K	Joback Method
tc	1234.25	K	Joback Method
tf	576.16	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.91	J/mol×K	1007.84	Joback Method
cpg	1164.84	J/mol×K	1045.58	Joback Method
cpg	1177.27	J/mol×K	1083.31	Joback Method
cpg	1188.26	J/mol×K	1121.05	Joback Method
cpg	1197.86	J/mol×K	1158.78	Joback Method
cpg	1206.13	J/mol×K	1196.52	Joback Method
cpg	1213.13	J/mol×K	1234.25	Joback Method

Sources

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=U380741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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