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

Inchi: InChI=1S/C23H35FO4/c1-2-3-12-18-27-22(25)15-8-6-4-5-7-9-16-23(26)28-19-17-20-13-1

InchiKey: KJQAVTXPVMXSNP-UHFFFAOYSA-N

Formula: C23H35FO4

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCCc1ccccc1F

Mol. weight [g/mol]: 394.52

Physical Properties

Property code	Value	Unit	Source
gf	-417.09	kJ/mol	Joback Method
hf	-978.70	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	87.22	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.766		Crippen Method
mcvol	327.820	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	909.15	K	Joback Method
tc	1113.70	K	Joback Method
tf	532.82	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.16	J/mol×K	909.15	Joback Method
cpg	1081.71	J/mol×K	943.24	Joback Method
cpg	1096.99	J/mol×K	977.33	Joback Method
cpg	1111.03	J/mol×K	1011.42	Joback Method
cpg	1123.86	J/mol×K	1045.51	Joback Method
cpg	1135.51	J/mol×K	1079.61	Joback Method
cpg	1146.01	J/mol×K	1113.70	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=U380746&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