Sebacic acid, hexyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C24H33F5O4/c1-3-4-5-12-15-32-17(30)13-10-8-6-7-9-11-14-18(31)33-16(2)19

InchiKey: QEPHAVQIBIRGAQ-UHFFFAOYSA-N

Formula: C24H33F5O4

SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 480.51

Physical Properties

Property code	Value	Unit	Source
gf	-1228.87	kJ/mol	Joback Method
hf	-1834.94	kJ/mol	Joback Method
hfus	67.46	kJ/mol	Joback Method
hvap	88.44	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	7.231		Crippen Method
mcvol	348.990	ml/mol	McGowan Method
pc	869.65	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	948.59	K	Joback Method
tc	1166.26	K	Joback Method
tf	581.53	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.18	J/mol×K	948.59	Joback Method
cpg	1168.40	J/mol×K	984.87	Joback Method
cpg	1183.09	J/mol×K	1021.15	Joback Method
cpg	1196.27	J/mol×K	1057.43	Joback Method
cpg	1207.97	J/mol×K	1093.70	Joback Method
cpg	1218.20	J/mol×K	1129.98	Joback Method
cpg	1226.98	J/mol×K	1166.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380664&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