Sebacic acid, 2-(pentafluorophenoxy)ethyl pentyl ester

Inchi: InChI=1S/C23H31F5O5/c1-2-3-10-13-31-16(29)11-8-6-4-5-7-9-12-17(30)32-14-15-33-23

InchiKey: JTTVHAIQEHGQMJ-UHFFFAOYSA-N

Formula: C23H31F5O5

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 482.48

Physical Properties

Property code	Value	Unit	Source
gf	-1339.85	kJ/mol	Joback Method
hf	-1941.24	kJ/mol	Joback Method
hfus	69.58	kJ/mol	Joback Method
hvap	89.02	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.158		Crippen Method
mcvol	340.770	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	948.57	K	Joback Method
tc	1167.15	K	Joback Method
tf	607.49	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.78	J/mol×K	948.57	Joback Method
cpg	1135.20	J/mol×K	985.00	Joback Method
cpg	1149.01	J/mol×K	1021.43	Joback Method
cpg	1161.20	J/mol×K	1057.86	Joback Method
cpg	1171.79	J/mol×K	1094.29	Joback Method
cpg	1180.77	J/mol×K	1130.72	Joback Method
cpg	1188.14	J/mol×K	1167.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416783&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