Sebacic acid, hexyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C24H33F5O5/c1-2-3-4-11-14-32-17(30)12-9-7-5-6-8-10-13-18(31)33-15-16-34

InchiKey: NUDFNEDQVMIQPY-UHFFFAOYSA-N

Formula: C24H33F5O5

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

Mol. weight [g/mol]: 496.51

Physical Properties

Property code	Value	Unit	Source
gf	-1331.43	kJ/mol	Joback Method
hf	-1961.88	kJ/mol	Joback Method
hfus	72.17	kJ/mol	Joback Method
hvap	91.24	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.548		Crippen Method
mcvol	354.860	ml/mol	McGowan Method
pc	856.97	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	971.45	K	Joback Method
tc	1199.39	K	Joback Method
tf	618.76	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.61	J/mol×K	971.45	Joback Method
cpg	1196.44	J/mol×K	1009.44	Joback Method
cpg	1210.47	J/mol×K	1047.43	Joback Method
cpg	1222.69	J/mol×K	1085.42	Joback Method
cpg	1233.13	J/mol×K	1123.41	Joback Method
cpg	1241.77	J/mol×K	1161.40	Joback Method
cpg	1248.64	J/mol×K	1199.39	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=U416784&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