Sebacic acid, octyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C26H37F5O5/c1-2-3-4-5-10-13-16-34-19(32)14-11-8-6-7-9-12-15-20(33)35-17

InchiKey: JUUFVOWAHCHQRK-UHFFFAOYSA-N

Formula: C26H37F5O5

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

Mol. weight [g/mol]: 524.56

Physical Properties

Property code	Value	Unit	Source
gf	-1314.59	kJ/mol	Joback Method
hf	-2003.16	kJ/mol	Joback Method
hfus	77.35	kJ/mol	Joback Method
hvap	95.69	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.329		Crippen Method
mcvol	383.040	ml/mol	McGowan Method
pc	768.19	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	1017.21	K	Joback Method
tc	1267.93	K	Joback Method
tf	641.30	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1303.38	J/mol×K	1017.21	Joback Method
cpg	1320.02	J/mol×K	1059.00	Joback Method
cpg	1334.37	J/mol×K	1100.78	Joback Method
cpg	1346.44	J/mol×K	1142.57	Joback Method
cpg	1356.27	J/mol×K	1184.36	Joback Method
cpg	1363.86	J/mol×K	1226.14	Joback Method
cpg	1369.24	J/mol×K	1267.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416786&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

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