Sebacic acid, di(1-(pentafluorophenyl)ethyl) ester

Inchi: InChI=1S/C26H24F10O4/c1-11(15-17(27)21(31)25(35)22(32)18(15)28)39-13(37)9-7-5-3-

InchiKey: PDVAHHFWCFZLRA-UHFFFAOYSA-N

Formula: C26H24F10O4

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

Mol. weight [g/mol]: 590.45

Physical Properties

Property code	Value	Unit	Source
gf	-2124.26	kJ/mol	Joback Method
hf	-2682.87	kJ/mol	Joback Method
hfus	76.62	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-10.87		Crippen Method
logp	8.107		Crippen Method
mcvol	362.260	ml/mol	McGowan Method
pc	796.18	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	1041.84	K	Joback Method
tc	1299.14	K	Joback Method
tf	681.04	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1194.21	J/mol×K	1041.84	Joback Method
cpg	1206.51	J/mol×K	1084.72	Joback Method
cpg	1216.59	J/mol×K	1127.61	Joback Method
cpg	1224.46	J/mol×K	1170.49	Joback Method
cpg	1230.13	J/mol×K	1213.37	Joback Method
cpg	1233.62	J/mol×K	1256.26	Joback Method
cpg	1234.94	J/mol×K	1299.14	Joback Method

Sources

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=U380667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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