Sebacic acid, di(2-(pentafluorophenoxy)ethyl) ester

Inchi: InChI=1S/C26H24F10O6/c27-15-17(29)21(33)25(22(34)18(15)30)41-11-9-39-13(37)7-5-3

InchiKey: KKVWNYRSUPTDOU-UHFFFAOYSA-N

Formula: C26H24F10O6

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

Mol. weight [g/mol]: 622.45

Physical Properties

Property code	Value	Unit	Source
gf	-2329.38	kJ/mol	Joback Method
hf	-2936.75	kJ/mol	Joback Method
hfus	86.04	kJ/mol	Joback Method
hvap	99.60	kJ/mol	Joback Method
log10ws	-9.42		Crippen Method
logp	6.743		Crippen Method
mcvol	374.000	ml/mol	McGowan Method
pc	774.18	kPa	Joback Method
rinpol	2902.00		NIST Webbook
rinpol	2902.00		NIST Webbook
tb	1087.56	K	Joback Method
tc	1380.38	K	Joback Method
tf	755.50	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1241.72	J/mol×K	1087.56	Joback Method
cpg	1251.22	J/mol×K	1136.36	Joback Method
cpg	1257.20	J/mol×K	1185.17	Joback Method
cpg	1259.59	J/mol×K	1233.97	Joback Method
cpg	1258.33	J/mol×K	1282.77	Joback Method
cpg	1253.37	J/mol×K	1331.57	Joback Method
cpg	1244.65	J/mol×K	1380.38	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=U416788&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