Sebacic acid, heptyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C25H35F5O4/c1-3-4-5-10-13-16-33-18(31)14-11-8-6-7-9-12-15-19(32)34-17(2

InchiKey: AQGFBYBXBFQIGU-UHFFFAOYSA-N

Formula: C25H35F5O4

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

Mol. weight [g/mol]: 494.54

Physical Properties

Property code	Value	Unit	Source
gf	-1220.45	kJ/mol	Joback Method
hf	-1855.58	kJ/mol	Joback Method
hfus	70.05	kJ/mol	Joback Method
hvap	90.67	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	7.621		Crippen Method
mcvol	363.080	ml/mol	McGowan Method
pc	822.42	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	971.47	K	Joback Method
tc	1198.19	K	Joback Method
tf	592.80	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.54	J/mol×K	971.47	Joback Method
cpg	1230.24	J/mol×K	1009.26	Joback Method
cpg	1245.23	J/mol×K	1047.04	Joback Method
cpg	1258.57	J/mol×K	1084.83	Joback Method
cpg	1270.26	J/mol×K	1122.61	Joback Method
cpg	1280.33	J/mol×K	1160.40	Joback Method
cpg	1288.83	J/mol×K	1198.19	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=U380665&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