Sebacic acid, 1-(pentafluorophenyl)ethyl propyl ester

Inchi: InChI=1S/C21H27F5O4/c1-3-12-29-14(27)10-8-6-4-5-7-9-11-15(28)30-13(2)16-17(22)19

InchiKey: DLZKCDUZUBDZIX-UHFFFAOYSA-N

Formula: C21H27F5O4

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

Mol. weight [g/mol]: 438.43

Physical Properties

Property code	Value	Unit	Source
gf	-1254.13	kJ/mol	Joback Method
hf	-1773.02	kJ/mol	Joback Method
hfus	59.69	kJ/mol	Joback Method
hvap	81.77	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.060		Crippen Method
mcvol	306.720	ml/mol	McGowan Method
pc	1038.57	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2327.00		NIST Webbook
tb	879.95	K	Joback Method
tc	1077.31	K	Joback Method
tf	547.72	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.21	J/mol×K	879.95	Joback Method
cpg	986.08	J/mol×K	912.84	Joback Method
cpg	999.80	J/mol×K	945.74	Joback Method
cpg	1012.38	J/mol×K	978.63	Joback Method
cpg	1023.82	J/mol×K	1011.52	Joback Method
cpg	1034.14	J/mol×K	1044.42	Joback Method
cpg	1043.33	J/mol×K	1077.31	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=U380661&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