Sebacic acid, butyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C22H29F5O4/c1-3-4-13-30-15(28)11-9-7-5-6-8-10-12-16(29)31-14(2)17-18(23

InchiKey: BKOWYFGYFGIDRE-UHFFFAOYSA-N

Formula: C22H29F5O4

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

Mol. weight [g/mol]: 452.46

Physical Properties

Property code	Value	Unit	Source
gf	-1245.71	kJ/mol	Joback Method
hf	-1793.66	kJ/mol	Joback Method
hfus	62.28	kJ/mol	Joback Method
hvap	83.99	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	6.450		Crippen Method
mcvol	320.810	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		NIST Webbook
tb	902.83	K	Joback Method
tc	1105.91	K	Joback Method
tf	558.99	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.95	J/mol×K	902.83	Joback Method
cpg	1046.26	J/mol×K	936.68	Joback Method
cpg	1060.31	J/mol×K	970.52	Joback Method
cpg	1073.11	J/mol×K	1004.37	Joback Method
cpg	1084.68	J/mol×K	1038.22	Joback Method
cpg	1095.02	J/mol×K	1072.06	Joback Method
cpg	1104.14	J/mol×K	1105.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380662&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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