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

Inchi: InChI=1S/C20H12F10O4/c1-5(9-11(21)15(25)19(29)16(26)12(9)22)33-7(31)3-4-8(32)34-

InchiKey: DDVHAYJWVFOKEN-UHFFFAOYSA-N

Formula: C20H12F10O4

SMILES: CC(OC(=O)CCC(=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]: 506.29

Physical Properties

Property code	Value	Unit	Source
gf	-2174.78	kJ/mol	Joback Method
hf	-2559.03	kJ/mol	Joback Method
hfus	61.08	kJ/mol	Joback Method
hvap	80.65	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	5.766		Crippen Method
mcvol	277.720	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	904.56	K	Joback Method
tc	1107.53	K	Joback Method
tf	613.42	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.83	J/mol×K	904.56	Joback Method
cpg	854.31	J/mol×K	938.39	Joback Method
cpg	863.67	J/mol×K	972.22	Joback Method
cpg	871.90	J/mol×K	1006.05	Joback Method
cpg	878.98	J/mol×K	1039.88	Joback Method
cpg	884.91	J/mol×K	1073.70	Joback Method
cpg	889.68	J/mol×K	1107.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380839&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