Succinic acid, ethyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C14H13F5O4/c1-3-22-7(20)4-5-8(21)23-6(2)9-10(15)12(17)14(19)13(18)11(9)1

InchiKey: OVUCRNDGRPPRSX-UHFFFAOYSA-N

Formula: C14H13F5O4

SMILES: CCOC(=O)CCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 340.24

Physical Properties

Property code	Value	Unit	Source
gf	-1313.07	kJ/mol	Joback Method
hf	-1628.54	kJ/mol	Joback Method
hfus	41.56	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.330		Crippen Method
mcvol	208.090	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook
tb	719.79	K	Joback Method
tc	899.93	K	Joback Method
tf	468.83	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.00	J/mol×K	719.79	Joback Method
cpg	587.63	J/mol×K	749.81	Joback Method
cpg	598.62	J/mol×K	779.84	Joback Method
cpg	608.96	J/mol×K	809.86	Joback Method
cpg	618.63	J/mol×K	839.88	Joback Method
cpg	627.64	J/mol×K	869.91	Joback Method
cpg	635.98	J/mol×K	899.93	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=U380820&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