Succinic acid, ethyl pentafluorophenyl ester

Inchi: InChI=1S/C12H9F5O4/c1-2-20-5(18)3-4-6(19)21-12-10(16)8(14)7(13)9(15)11(12)17/h2-4
InchiKey: UJJIVIIWNPPMNN-UHFFFAOYSA-N
Formula: C12H9F5O4
SMILES: CCOC(=O)CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 312.19

Physical Properties

Property code	Value	Unit	Source
gf	-1327.47	kJ/mol	Joback Method
hf	-1581.98	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.631		Crippen Method
mcvol	179.910	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
tb	674.47	K	Joback Method
tc	852.73	K	Joback Method
tf	461.29	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.39	J/mol×K	674.47	Joback Method
cpg	482.64	J/mol×K	704.18	Joback Method
cpg	492.37	J/mol×K	733.89	Joback Method
cpg	501.59	J/mol×K	763.60	Joback Method
cpg	510.27	J/mol×K	793.31	Joback Method
cpg	518.41	J/mol×K	823.02	Joback Method
cpg	526.00	J/mol×K	852.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390360&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

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