Succinic acid, ethyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C13H12F4O4/c1-2-20-9(18)3-4-10(19)21-6-7-5-8(14)12(16)13(17)11(7)15/h5H

InchiKey: OEUICBCILZUNEB-UHFFFAOYSA-N

Formula: C13H12F4O4

SMILES: CCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 308.23

Physical Properties

Property code	Value	Unit	Source
gf	-1114.61	kJ/mol	Joback Method
hf	-1395.04	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.630		Crippen Method
mcvol	192.230	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1671.00		NIST Webbook
tb	693.10	K	Joback Method
tc	875.69	K	Joback Method
tf	459.45	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.41	J/mol×K	693.10	Joback Method
cpg	527.81	J/mol×K	723.53	Joback Method
cpg	538.61	J/mol×K	753.96	Joback Method
cpg	548.78	J/mol×K	784.39	Joback Method
cpg	558.33	J/mol×K	814.82	Joback Method
cpg	567.26	J/mol×K	845.26	Joback Method
cpg	575.54	J/mol×K	875.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381610&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