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

Inchi: InChI=1S/C21H28F4O4/c1-2-3-4-5-6-7-8-9-12-28-17(26)10-11-18(27)29-14-15-13-16(22
InchiKey: PLDSZLDFNBIKJL-UHFFFAOYSA-N
Formula: C21H28F4O4
SMILES: CCCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 420.44

Physical Properties

Property code	Value	Unit	Source
gf	-1047.25	kJ/mol	Joback Method
hf	-1560.16	kJ/mol	Joback Method
hfus	60.52	kJ/mol	Joback Method
hvap	82.31	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.750		Crippen Method
mcvol	304.950	ml/mol	McGowan Method
pc	1074.28	kPa	Joback Method
rinpol	2442.00		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	876.14	K	Joback Method
tc	1072.72	K	Joback Method
tf	549.61	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.21	J/mol×K	876.14	Joback Method
cpg	979.30	J/mol×K	908.90	Joback Method
cpg	993.27	J/mol×K	941.67	Joback Method
cpg	1006.11	J/mol×K	974.43	Joback Method
cpg	1017.86	J/mol×K	1007.20	Joback Method
cpg	1028.51	J/mol×K	1039.96	Joback Method
cpg	1038.08	J/mol×K	1072.72	Joback Method

Sources

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=U381620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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