Succinic acid, dodec-2-en-1-yl pentafluorophenyl ester

Inchi: InChI=1S/C22H27F5O4/c1-2-3-4-5-6-7-8-9-10-11-14-30-15(28)12-13-16(29)31-22-20(26
InchiKey: MUWYEKYACVBWLP-ZHACJKMWSA-N
Formula: C22H27F5O4
SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 450.44

Physical Properties

Property code	Value	Unit	Source
gf	-1163.05	kJ/mol	Joback Method
hf	-1671.16	kJ/mol	Joback Method
hfus	66.01	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.308		Crippen Method
mcvol	316.510	ml/mol	McGowan Method
pc	1004.62	kPa	Joback Method
rinpol	2397.00		NIST Webbook
rinpol	2397.00		NIST Webbook
tb	907.43	K	Joback Method
tc	1111.31	K	Joback Method
tf	568.91	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.81	J/mol×K	907.43	Joback Method
cpg	1017.59	J/mol×K	941.41	Joback Method
cpg	1031.23	J/mol×K	975.39	Joback Method
cpg	1043.75	J/mol×K	1009.37	Joback Method
cpg	1055.18	J/mol×K	1043.35	Joback Method
cpg	1065.53	J/mol×K	1077.33	Joback Method
cpg	1074.83	J/mol×K	1111.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390357&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