Succinic acid, heptyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C19H23F5O5/c1-2-3-4-5-6-9-27-12(25)7-8-13(26)28-10-11-29-19-17(23)15(21
InchiKey: GRBLFPIZQGOTEG-UHFFFAOYSA-N
Formula: C19H23F5O5
SMILES: CCCCCCCOC(=O)CCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 426.37

Physical Properties

Property code	Value	Unit	Source
gf	-1373.53	kJ/mol	Joback Method
hf	-1858.68	kJ/mol	Joback Method
hfus	59.22	kJ/mol	Joback Method
hvap	80.11	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.598		Crippen Method
mcvol	284.410	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	857.05	K	Joback Method
tc	1049.45	K	Joback Method
tf	562.41	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.73	J/mol×K	857.05	Joback Method
cpg	895.48	J/mol×K	889.12	Joback Method
cpg	908.15	J/mol×K	921.18	Joback Method
cpg	919.75	J/mol×K	953.25	Joback Method
cpg	930.27	J/mol×K	985.31	Joback Method
cpg	939.69	J/mol×K	1017.38	Joback Method
cpg	948.01	J/mol×K	1049.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381553&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