Succinic acid, 2-methylhex-3-yl 2-(pentafluorophenoxy)ethyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-1378.41	kJ/mol	Joback Method
hf	-1869.24	kJ/mol	Joback Method
hfus	52.18	kJ/mol	Joback Method
hvap	79.33	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.452		Crippen Method
mcvol	284.410	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	856.17	K	Joback Method
tc	1049.08	K	Joback Method
tf	532.41	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.79	J/mol×K	856.17	Joback Method
cpg	896.55	J/mol×K	888.32	Joback Method
cpg	909.22	J/mol×K	920.47	Joback Method
cpg	920.78	J/mol×K	952.63	Joback Method
cpg	931.24	J/mol×K	984.78	Joback Method
cpg	940.57	J/mol×K	1016.93	Joback Method
cpg	948.78	J/mol×K	1049.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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