Succinic acid, octyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C20H25F5O5/c1-2-3-4-5-6-7-10-28-13(26)8-9-14(27)29-11-12-30-20-18(24)16
InchiKey: FGPSZABEIOCBAC-UHFFFAOYSA-N
Formula: C20H25F5O5
SMILES: CCCCCCCCOC(=O)CCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 440.40

Physical Properties

Property code	Value	Unit	Source
gf	-1365.11	kJ/mol	Joback Method
hf	-1879.32	kJ/mol	Joback Method
hfus	61.81	kJ/mol	Joback Method
hvap	82.34	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.988		Crippen Method
mcvol	298.500	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	879.93	K	Joback Method
tc	1077.35	K	Joback Method
tf	573.68	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.32	J/mol×K	879.93	Joback Method
cpg	954.49	J/mol×K	912.83	Joback Method
cpg	967.48	J/mol×K	945.74	Joback Method
cpg	979.28	J/mol×K	978.64	Joback Method
cpg	989.90	J/mol×K	1011.54	Joback Method
cpg	999.32	J/mol×K	1044.45	Joback Method
cpg	1007.53	J/mol×K	1077.35	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=U381554&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