Succinic acid, isobutyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C16H17F5O5/c1-8(2)7-26-10(23)4-3-9(22)24-5-6-25-16-14(20)12(18)11(17)13

InchiKey: YPRYTYREFORBNK-UHFFFAOYSA-N

Formula: C16H17F5O5

SMILES: CC(C)COC(=O)CCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 384.30

Physical Properties

Property code	Value	Unit	Source
gf	-1401.23	kJ/mol	Joback Method
hf	-1802.04	kJ/mol	Joback Method
hfus	47.93	kJ/mol	Joback Method
hvap	73.05	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.284		Crippen Method
mcvol	242.140	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	787.97	K	Joback Method
tc	971.51	K	Joback Method
tf	513.60	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.28	J/mol×K	787.97	Joback Method
cpg	723.78	J/mol×K	818.56	Joback Method
cpg	735.45	J/mol×K	849.15	Joback Method
cpg	746.28	J/mol×K	879.74	Joback Method
cpg	756.26	J/mol×K	910.33	Joback Method
cpg	765.37	J/mol×K	940.92	Joback Method
cpg	773.61	J/mol×K	971.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381548&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