Succinic acid, butyl 2-(pentafluorophenoxy)ethyl ester

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

InchiKey: YCXGXZLCQQSUFX-UHFFFAOYSA-N

Formula: C16H17F5O5

SMILES: CCCCOC(=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	-1398.79	kJ/mol	Joback Method
hf	-1796.76	kJ/mol	Joback Method
hfus	51.45	kJ/mol	Joback Method
hvap	73.43	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.428		Crippen Method
mcvol	242.140	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	788.41	K	Joback Method
tc	970.80	K	Joback Method
tf	528.60	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.72	J/mol×K	788.41	Joback Method
cpg	723.13	J/mol×K	818.81	Joback Method
cpg	734.73	J/mol×K	849.21	Joback Method
cpg	745.52	J/mol×K	879.60	Joback Method
cpg	755.48	J/mol×K	910.00	Joback Method
cpg	764.58	J/mol×K	940.40	Joback Method
cpg	772.84	J/mol×K	970.80	Joback Method

Sources

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=U381549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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