Succinic acid, 3,5-dimethylphenyl pentafluorobenzyl ester

Inchi: InChI=1S/C19H15F5O4/c1-9-5-10(2)7-11(6-9)28-14(26)4-3-13(25)27-8-12-15(20)17(22)
InchiKey: CUMMRWWEDFRGDN-UHFFFAOYSA-N
Formula: C19H15F5O4
SMILES: Cc1cc(C)cc(OC(=O)CCC(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 402.31

Physical Properties

Property code	Value	Unit	Source
gf	-1175.38	kJ/mol	Joback Method
hf	-1512.87	kJ/mol	Joback Method
hfus	51.30	kJ/mol	Joback Method
hvap	81.30	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	4.428		Crippen Method
mcvol	254.780	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
tb	871.27	K	Joback Method
tc	1074.93	K	Joback Method
tf	591.64	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.81	J/mol×K	871.27	Joback Method
cpg	765.22	J/mol×K	905.21	Joback Method
cpg	775.60	J/mol×K	939.16	Joback Method
cpg	784.94	J/mol×K	973.10	Joback Method
cpg	793.25	J/mol×K	1007.05	Joback Method
cpg	800.52	J/mol×K	1040.99	Joback Method
cpg	806.76	J/mol×K	1074.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360731&Units=SI

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