Succinic acid, 3,5-difluorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H9F7O4/c18-7-3-8(19)5-9(4-7)28-12(26)2-1-11(25)27-6-10-13(20)15(22)17

InchiKey: UPICAGKAPFTBFD-UHFFFAOYSA-N

Formula: C17H9F7O4

SMILES: O=C(CCC(=O)Oc1cc(F)cc(F)c1)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 410.24

Physical Properties

Property code	Value	Unit	Source
gf	-1581.84	kJ/mol	Joback Method
hf	-1863.81	kJ/mol	Joback Method
hfus	52.28	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	4.089		Crippen Method
mcvol	230.140	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	2115.00		NIST Webbook
tb	824.05	K	Joback Method
tc	1017.91	K	Joback Method
tf	570.28	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.64	J/mol×K	824.05	Joback Method
cpg	667.77	J/mol×K	856.36	Joback Method
cpg	677.06	J/mol×K	888.67	Joback Method
cpg	685.50	J/mol×K	920.98	Joback Method
cpg	693.10	J/mol×K	953.29	Joback Method
cpg	699.84	J/mol×K	985.60	Joback Method
cpg	705.73	J/mol×K	1017.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358035&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