Succinic acid, 4-chloro-3-methylphenyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H12ClF5O4/c1-8-6-9(2-3-11(8)19)28-13(26)5-4-12(25)27-7-10-14(20)16(22
InchiKey: FOAVMNZUCOBSSC-UHFFFAOYSA-N
Formula: C18H12ClF5O4
SMILES: Cc1cc(OC(=O)CCC(=O)OCc2c(F)c(F)c(F)c(F)c2F)ccc1Cl
Mol. weight [g/mol]: 422.73

Physical Properties

Property code	Value	Unit	Source
gf	-1195.73	kJ/mol	Joback Method
hf	-1507.97	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	83.46	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	4.773		Crippen Method
mcvol	252.930	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	885.82	K	Joback Method
tc	1093.67	K	Joback Method
tf	610.29	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.15	J/mol×K	885.82	Joback Method
cpg	729.15	J/mol×K	920.46	Joback Method
cpg	738.15	J/mol×K	955.10	Joback Method
cpg	746.13	J/mol×K	989.75	Joback Method
cpg	753.09	J/mol×K	1024.39	Joback Method
cpg	759.03	J/mol×K	1059.03	Joback Method
cpg	763.94	J/mol×K	1093.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389890&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