Succinic acid, phenyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H11F5O4/c18-13-10(14(19)16(21)17(22)15(13)20)8-25-11(23)6-7-12(24)2
InchiKey: PVNQTJMLDZDVHK-UHFFFAOYSA-N
Formula: C17H11F5O4
SMILES: O=C(CCC(=O)Oc1ccccc1)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 374.26

Physical Properties

Property code	Value	Unit	Source
gf	-1172.96	kJ/mol	Joback Method
hf	-1448.65	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	75.52	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	3.811		Crippen Method
mcvol	226.600	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	815.55	K	Joback Method
tc	1016.26	K	Joback Method
tf	544.06	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.43	J/mol×K	815.55	Joback Method
cpg	656.37	J/mol×K	849.00	Joback Method
cpg	666.40	J/mol×K	882.45	Joback Method
cpg	675.53	J/mol×K	915.90	Joback Method
cpg	683.76	J/mol×K	949.36	Joback Method
cpg	691.09	J/mol×K	982.81	Joback Method
cpg	697.53	J/mol×K	1016.26	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=U357997&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