Succinic acid, 2-chlorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H10ClF5O4/c18-9-3-1-2-4-10(9)27-12(25)6-5-11(24)26-7-8-13(19)15(21)1

InchiKey: UNQIQIILSGPMIJ-UHFFFAOYSA-N

Formula: C17H10ClF5O4

SMILES: O=C(CCC(=O)Oc1ccccc1Cl)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 408.70

Physical Properties

Property code	Value	Unit	Source
gf	-1194.52	kJ/mol	Joback Method
hf	-1475.86	kJ/mol	Joback Method
hfus	50.70	kJ/mol	Joback Method
hvap	80.57	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.465		Crippen Method
mcvol	238.840	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2323.00		NIST Webbook
tb	857.96	K	Joback Method
tc	1064.21	K	Joback Method
tf	586.50	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.41	J/mol×K	857.96	Joback Method
cpg	675.19	J/mol×K	892.33	Joback Method
cpg	684.03	J/mol×K	926.71	Joback Method
cpg	691.93	J/mol×K	961.08	Joback Method
cpg	698.89	J/mol×K	995.46	Joback Method
cpg	704.91	J/mol×K	1029.83	Joback Method
cpg	709.99	J/mol×K	1064.21	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=U357552&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