Succinic acid, 2,3-dichlorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H9Cl2F5O4/c18-8-2-1-3-9(12(8)19)28-11(26)5-4-10(25)27-6-7-13(20)15(22
InchiKey: HUAOMEIAKQEZEL-UHFFFAOYSA-N
Formula: C17H9Cl2F5O4
SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 443.15

Physical Properties

Property code	Value	Unit	Source
gf	-1216.08	kJ/mol	Joback Method
hf	-1503.07	kJ/mol	Joback Method
hfus	54.51	kJ/mol	Joback Method
hvap	85.62	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.118		Crippen Method
mcvol	251.080	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	900.37	K	Joback Method
tc	1112.47	K	Joback Method
tf	628.94	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.29	J/mol×K	900.37	Joback Method
cpg	691.88	J/mol×K	935.72	Joback Method
cpg	699.49	J/mol×K	971.07	Joback Method
cpg	706.10	J/mol×K	1006.42	Joback Method
cpg	711.71	J/mol×K	1041.77	Joback Method
cpg	716.32	J/mol×K	1077.12	Joback Method
cpg	719.93	J/mol×K	1112.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389891&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