

Succinic acid, 2,4,6-trichlorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H8Cl3F5O4/c18-6-3-8(19)17(9(20)4-6)29-11(27)2-1-10(26)28-5-7-12(21)14-13
InchiKey: SEKHNV00YYWZKW-UHFFFAOYSA-N
Formula: C17H8Cl3F5O4
SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 477.59

Physical Properties

Property code	Value	Unit	Source
gf	-1237.64	kJ/mol	Joback Method
hf	-1530.28	kJ/mol	Joback Method
hfus	58.32	kJ/mol	Joback Method
hvap	90.67	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	5.771		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook
tb	942.78	K	Joback Method
tc	1161.15	K	Joback Method
tf	671.38	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.12	J/molxK	942.78	Joback Method
cpg	706.47	J/molxK	979.18	Joback Method
cpg	712.77	J/molxK	1015.57	Joback Method
cpg	718.00	J/molxK	1051.97	Joback Method
cpg	722.16	J/molxK	1088.36	Joback Method
cpg	725.24	J/molxK	1124.76	Joback Method
cpg	727.23	J/molxK	1161.15	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=U389893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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