Succinic acid, 3-methylbut-2-yl pentachlorophenyl ester

Inchi: InChI=1S/C15H15Cl5O4/c1-6(2)7(3)23-8(21)4-5-9(22)24-15-13(19)11(17)10(16)12(18)14

InchiKey: OKMHWKLWJBPDRX-UHFFFAOYSA-N

Formula: C15H15Cl5O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 436.54

Physical Properties

Property code	Value	Unit	Source
gf	-392.69	kJ/mol	Joback Method
hf	-752.61	kJ/mol	Joback Method
hfus	46.21	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.227		Crippen Method
mcvol	274.530	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	933.03	K	Joback Method
tc	1163.39	K	Joback Method
tf	611.75	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.14	J/mol×K	933.03	Joback Method
cpg	735.33	J/mol×K	1124.99	Joback Method
cpg	730.96	J/mol×K	1086.60	Joback Method
cpg	725.46	J/mol×K	1048.21	Joback Method
cpg	718.81	J/mol×K	1009.82	Joback Method
cpg	711.04	J/mol×K	971.42	Joback Method
cpg	738.54	J/mol×K	1163.39	Joback Method
dvisc	0.0000464	Pa×s	933.03	Joback Method

dvisc	0.0000571	Pa×s	879.48	Joback Method
dvisc	0.0000721	Pa×s	825.94	Joback Method
dvisc	0.0000941	Pa×s	772.39	Joback Method
dvisc	0.0001277	Pa×s	718.84	Joback Method
dvisc	0.0001821	Pa×s	665.30	Joback Method
dvisc	0.0002762	Pa×s	611.75	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=U390046&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
dvisc:	Dynamic viscosity
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