

Succinic acid, di(2,3,5,6-tetrachlorophenyl) ester

Inchi:	InChI=1S/C16H6Cl8O4/c17-5-3-6(18)12(22)15(11(5)21)27-9(25)1-2-10(26)28-16-13(23)
InchiKey:	OZGKXYXDIJDTQO-UHFFFAOYSA-N
Formula:	C16H6Cl8O4
SMILES:	O=C(CCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	545.84

Physical Properties

Property code	Value	Unit	Source
gf	-331.66	kJ/mol	Joback Method
hf	-607.79	kJ/mol	Joback Method
hfus	61.32	kJ/mol	Joback Method
hvap	114.45	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	8.205		Crippen Method
mcvol	301.580	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	3486.00		NIST Webbook
rinpol	3486.00		NIST Webbook
tb	1110.70	K	Joback Method
tc	1373.95	K	Joback Method
tf	806.76	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.23	J/mol×K	1110.70	Joback Method
cpg	670.10	J/mol×K	1330.08	Joback Method
cpg	673.96	J/mol×K	1286.20	Joback Method
cpg	676.39	J/mol×K	1242.33	Joback Method
cpg	677.41	J/mol×K	1198.45	Joback Method
cpg	677.01	J/mol×K	1154.58	Joback Method
cpg	664.79	J/mol×K	1373.95	Joback Method
dvisc	0.0000323	Paxs	1110.70	Joback Method

dvisc	0.0000376	Paxs	1060.04	Joback Method
dvisc	0.0000446	Paxs	1009.39	Joback Method
dvisc	0.0000538	Paxs	958.73	Joback Method
dvisc	0.0000662	Paxs	908.07	Joback Method
dvisc	0.0000836	Paxs	857.42	Joback Method
dvisc	0.0001087	Paxs	806.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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