

Succinic acid, ethyl 2,3,4,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C12H10Cl4O4/c1-2-19-8(17)3-4-9(18)20-12-7(14)5-6(13)10(15)11(12)16/h5H,1
InchiKey:	JDEADFKPUSQYMO-UHFFFAOYSA-N
Formula:	C12H10Cl4O4
SMILES:	CCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	360.02

Physical Properties

Property code	Value	Unit	Source
gf	-391.51	kJ/mol	Joback Method
hf	-652.92	kJ/mol	Joback Method
hfus	41.68	kJ/mol	Joback Method
hvap	83.08	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.549		Crippen Method
mcvol	220.020	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinqol	2252.00		NIST Webbook
tb	822.86	K	Joback Method
tc	1049.22	K	Joback Method
tf	565.50	K	Joback Method
vc	0.844	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.18	J/molxK	822.86	Joback Method
cpg	530.17	J/molxK	860.59	Joback Method
cpg	538.31	J/molxK	898.31	Joback Method
cpg	545.57	J/molxK	936.04	Joback Method
cpg	551.94	J/molxK	973.76	Joback Method
cpg	557.43	J/molxK	1011.49	Joback Method
cpg	562.01	J/molxK	1049.22	Joback Method
dvisc	0.0004334	Paxs	565.50	Joback Method
dvisc	0.0003099	Paxs	608.39	Joback Method

dvisc	0.0002316	Paxs	651.29	Joback Method
dvisc	0.0001794	Paxs	694.18	Joback Method
dvisc	0.0001432	Paxs	737.07	Joback Method
dvisc	0.0001171	Paxs	779.97	Joback Method
dvisc	0.0000979	Paxs	822.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U349673&Units=SI

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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