

Succinic acid, 3-chlorophenyl 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C16H10Cl4O4/c17-9-2-1-3-10(6-9)23-15(21)4-5-16(22)24-14-8-12(19)11(18)7-
InchiKey:	LDSJVMXFUQAFEY-UHFFFAOYSA-N
Formula:	C16H10Cl4O4
SMILES:	O=C(CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	408.06

Physical Properties

Property code	Value	Unit	Source
gf	-245.42	kJ/mol	Joback Method
hf	-498.95	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	94.26	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.591		Crippen Method
mvol	252.620	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	941.06	K	Joback Method
tc	1188.49	K	Joback Method
tf	637.00	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.85	J/molxK	941.06	Joback Method
cpg	640.69	J/molxK	982.30	Joback Method
cpg	647.35	J/molxK	1023.54	Joback Method
cpg	652.84	J/molxK	1064.78	Joback Method
cpg	657.18	J/molxK	1106.01	Joback Method
cpg	660.38	J/molxK	1147.25	Joback Method
cpg	662.46	J/molxK	1188.49	Joback Method
dvisc	0.0002777	Paxs	637.00	Joback Method

dvisc	0.0001940	Paxs	687.68	Joback Method
dvisc	0.0001424	Paxs	738.35	Joback Method
dvisc	0.0001087	Paxs	789.03	Joback Method
dvisc	0.0000858	Paxs	839.71	Joback Method
dvisc	0.0000695	Paxs	890.38	Joback Method
dvisc	0.0000576	Paxs	941.06	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=U389971&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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