

Succinic acid, 2,4,6-trichlorophenyl 4-chloro-2-methylphenyl ester

Inchi:	InChI=1S/C17H12Cl4O4/c1-9-6-10(18)2-3-14(9)24-15(22)4-5-16(23)25-17-12(20)7-11(19)
InchiKey:	LBQSJXNKQLETLF-UHFFFAOYSA-N
Formula:	C17H12Cl4O4
SMILES:	<chem>Cc1cc(Cl)ccc1OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl</chem>
Mol. weight [g/mol]:	422.09

Physical Properties

Property code	Value	Unit	Source
gf	-246.63	kJ/mol	Joback Method
hf	-531.06	kJ/mol	Joback Method
hfus	48.29	kJ/mol	Joback Method
hvap	97.15	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.900		Crippen Method
mvol	266.710	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2875.00		NIST Webbook
rinpol	2875.00		NIST Webbook
tb	968.92	K	Joback Method
tc	1214.51	K	Joback Method
tf	660.79	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.12	J/molxK	968.92	Joback Method
cpg	694.03	J/molxK	1009.85	Joback Method
cpg	700.69	J/molxK	1050.78	Joback Method
cpg	706.12	J/molxK	1091.71	Joback Method
cpg	710.32	J/molxK	1132.64	Joback Method
cpg	713.31	J/molxK	1173.57	Joback Method
cpg	715.10	J/molxK	1214.51	Joback Method
dvisc	0.0002316	Paxs	660.79	Joback Method

dvisc	0.0001643	Paxs	712.15	Joback Method
dvisc	0.0001221	Paxs	763.50	Joback Method
dvisc	0.0000942	Paxs	814.86	Joback Method
dvisc	0.0000749	Paxs	866.21	Joback Method
dvisc	0.0000612	Paxs	917.57	Joback Method
dvisc	0.0000510	Paxs	968.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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