

Succinic acid, 2-chlorophenyl 2,4-dichloro-6-formylphenyl ester

Inchi:	InChI=1S/C17H11Cl3O5/c18-11-7-10(9-21)17(13(20)8-11)25-16(23)6-5-15(22)24-14-4-2
InchiKey:	SZMJPF0XJBXXNA-UHFFFAOYSA-N
Formula:	C17H11Cl3O5
SMILES:	O=Cc1cc(Cl)cc(Cl)c1OC(=O)CCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	401.62

Physical Properties

Property code	Value	Unit	Source
gf	-324.59	kJ/mol	Joback Method
hf	-589.43	kJ/mol	Joback Method
hfus	46.77	kJ/mol	Joback Method
hvap	98.82	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	4.750		Crippen Method
mcvol	256.040	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinsol	2966.00		NIST Webbook
tb	975.17	K	Joback Method
tc	1219.38	K	Joback Method
tf	660.35	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.23	J/molxK	975.17	Joback Method
cpg	697.37	J/molxK	1178.68	Joback Method
cpg	694.92	J/molxK	1137.98	Joback Method
cpg	691.30	J/molxK	1097.28	Joback Method
cpg	686.49	J/molxK	1056.57	Joback Method
cpg	680.47	J/molxK	1015.87	Joback Method
cpg	698.66	J/molxK	1219.38	Joback Method
dvisc	0.0000629	Paxs	975.17	Joback Method
dvisc	0.0000759	Paxs	922.70	Joback Method

dvisc	0.0000937	Paxs	870.23	Joback Method
dvisc	0.0001187	Paxs	817.76	Joback Method
dvisc	0.0001555	Paxs	765.29	Joback Method
dvisc	0.0002118	Paxs	712.82	Joback Method
dvisc	0.0003032	Paxs	660.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357556&Units=SI
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

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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