

Succinic acid, 2,4,6-trichlorophenyl 3-phenylpropyl ester

Inchi:	InChI=1S/C19H17Cl3O4/c20-14-11-15(21)19(16(22)12-14)26-18(24)9-8-17(23)25-10-4-7
InchiKey:	NVVCWJKTNAAUTQ-UHFFFAOYSA-N
Formula:	C19H17Cl3O4
SMILES:	O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCCc1ccccc1
Mol. weight [g/mol]:	415.69

Physical Properties

Property code	Value	Unit	Source
gf	-198.60	kJ/mol	Joback Method
hf	-533.66	kJ/mol	Joback Method
hfus	50.05	kJ/mol	Joback Method
hvap	95.89	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.508		Crippen Method
mvol	282.650	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	3010.00		NIST Webbook
rinpol	3010.00		NIST Webbook
tb	967.29	K	Joback Method
tc	1204.77	K	Joback Method
tf	628.37	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.07	J/molxK	967.29	Joback Method
cpg	821.73	J/molxK	1165.19	Joback Method
cpg	816.76	J/molxK	1125.61	Joback Method
cpg	810.65	J/molxK	1086.03	Joback Method
cpg	803.35	J/molxK	1046.45	Joback Method
cpg	794.84	J/molxK	1006.87	Joback Method
cpg	825.57	J/molxK	1204.77	Joback Method
dvisc	0.0000427	Paxs	967.29	Joback Method

dvisc	0.0000526	Paxs	910.80	Joback Method
dvisc	0.0000667	Paxs	854.32	Joback Method
dvisc	0.0000874	Paxs	797.83	Joback Method
dvisc	0.0001193	Paxs	741.34	Joback Method
dvisc	0.0001716	Paxs	684.86	Joback Method
dvisc	0.0002633	Paxs	628.37	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=U389736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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