

Succinic acid, 3-chlorophenyl 3-phenylprop-2-en-1-yl ester

Inchi:	InChI=1S/C19H17ClO4/c20-16-9-4-10-17(14-16)24-19(22)12-11-18(21)23-13-5-8-15-6-2
InchiKey:	CIVQBGWYHIENPB-VMPITWQZSA-N
Formula:	C19H17ClO4
SMILES:	O=C(CCC(=O)Oc1cccc(Cl)c1)OCC=Cc1cccc1
Mol. weight [g/mol]:	344.79

Physical Properties

Property code	Value	Unit	Source
gf	-75.26	kJ/mol	Joback Method
hf	-362.02	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	85.76	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.282		Crippen Method
mvol	253.870	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	886.63	K	Joback Method
tc	1122.07	K	Joback Method
tf	538.41	K	Joback Method
vc	0.961	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.77	J/molxK	886.63	Joback Method
cpg	770.26	J/molxK	1082.83	Joback Method
cpg	762.25	J/molxK	1043.59	Joback Method
cpg	753.25	J/molxK	1004.35	Joback Method
cpg	743.22	J/molxK	965.11	Joback Method
cpg	732.08	J/molxK	925.87	Joback Method
cpg	777.35	J/molxK	1122.07	Joback Method
dvisc	0.0000489	Paxs	886.63	Joback Method

dvisc	0.0000620	Paxs	828.59	Joback Method
dvisc	0.0000814	Paxs	770.56	Joback Method
dvisc	0.0001118	Paxs	712.52	Joback Method
dvisc	0.0001624	Paxs	654.48	Joback Method
dvisc	0.0002536	Paxs	596.45	Joback Method
dvisc	0.0004361	Paxs	538.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391047&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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

Latest version available from:

<https://www.chemeo.com/cid/99-676-3/Succinic-acid-3-chlorophenyl-3-phenylprop-2-en-1-yl-ester.pdf>

Generated by Cheméo on 2024-04-29 06:51:32.914914481 +0000 UTC m=+16662741.835491793.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.