

Succinic acid, 3-chlorophenyl cis-hex-3-en-1-yl ester

Inchi:	InChI=1S/C16H19ClO4/c1-2-3-4-5-11-20-15(18)9-10-16(19)21-14-8-6-7-13(17)12-14/h3-
InchiKey:	SQRAYFATJYUVQL-ARJAWSKDSA-N
Formula:	C16H19ClO4
SMILES:	CCC=CCCOC(=O)CCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	310.77

Physical Properties

Property code	Value	Unit	Source
gf	-212.93	kJ/mol	Joback Method
hf	-536.63	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.925		Crippen Method
mvol	235.360	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	791.31	K	Joback Method
tc	1002.86	K	Joback Method
tf	478.18	K	Joback Method
vc	0.900	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.61	J/molxK	791.31	Joback Method
cpg	707.68	J/molxK	967.60	Joback Method
cpg	697.88	J/molxK	932.35	Joback Method
cpg	687.19	J/molxK	897.09	Joback Method
cpg	675.61	J/molxK	861.83	Joback Method
cpg	663.09	J/molxK	826.57	Joback Method
cpg	716.64	J/molxK	1002.86	Joback Method
dvisc	0.0000719	Paxs	791.31	Joback Method

dvisc	0.0000914	Paxs	739.12	Joback Method
dvisc	0.0001204	Paxs	686.93	Joback Method
dvisc	0.0001660	Paxs	634.75	Joback Method
dvisc	0.0002424	Paxs	582.56	Joback Method
dvisc	0.0003814	Paxs	530.37	Joback Method
dvisc	0.0006625	Paxs	478.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391087&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/118-430-3/Succinic-acid-3-chlorophenyl-cis-hex-3-en-1-yl-ester.pdf>

Generated by Cheméo on 2024-05-03 19:45:49.689934327 +0000 UTC m=+17054798.610511643.

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