

Succinic acid, 4-chloro-3-methylphenyl oct-1-en-3-yl ester

Inchi:	InChI=1S/C19H25ClO4/c1-4-6-7-8-15(5-2)23-18(21)11-12-19(22)24-16-9-10-17(20)14(3)
InchiKey:	PIMDWENCXPFRBC-UHFFFAOYSA-N
Formula:	C19H25ClO4
SMILES:	<chem>C=CC(CCCCC)OC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1</chem>
Mol. weight [g/mol]:	352.85

Physical Properties

Property code	Value	Unit	Source
gf	-192.12	kJ/mol	Joback Method
hf	-607.09	kJ/mol	Joback Method
hfus	43.20	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.012		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2513.00		NIST Webbook
tb	857.01	K	Joback Method
tc	1065.79	K	Joback Method
tf	512.83	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.44	J/molxK	857.01	Joback Method
cpg	879.17	J/molxK	1031.00	Joback Method
cpg	869.14	J/molxK	996.20	Joback Method
cpg	858.08	J/molxK	961.40	Joback Method
cpg	845.95	J/molxK	926.60	Joback Method
cpg	832.75	J/molxK	891.81	Joback Method
cpg	888.18	J/molxK	1065.79	Joback Method
dvisc	0.0000543	Paxs	857.01	Joback Method
dvisc	0.0000693	Paxs	799.65	Joback Method

dvisc	0.0000918	Paxs	742.28	Joback Method
dvisc	0.0001274	Paxs	684.92	Joback Method
dvisc	0.0001879	Paxs	627.56	Joback Method
dvisc	0.0002997	Paxs	570.19	Joback Method
dvisc	0.0005305	Paxs	512.83	Joback Method

Sources

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=U391323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/99-785-2/Succinic-acid-4-chloro-3-methylphenyl-oct-1-en-3-yl-ester.pdf>

Generated by Cheméo on 2024-04-29 10:19:17.108077149 +0000 UTC m=+16675206.028654460.

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