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

Inchi: InChI=1S/C20H27ClO4/c1-3-4-5-6-7-8-9-14-24-19(22)12-13-20(23)25-17-10-11-18(21)16

InchiKey: IANBKEXRTISLMI-BQYQJAHWSA-N

Formula: C20H27ClO4

SMILES: CCCCCC=CCCOC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 366.88

Physical Properties

Property code	Value	Unit	Source
gf	-188.88	kJ/mol	Joback Method
hf	-630.66	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	86.37	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.404		Crippen Method
mcvol	291.720	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	887.81	K	Joback Method
tc	1097.74	K	Joback Method
tf	535.78	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.67	J/mol×K	887.81	Joback Method
cpg	891.14	J/mol×K	922.80	Joback Method
cpg	904.52	J/mol×K	957.79	Joback Method
cpg	916.85	J/mol×K	992.78	Joback Method
cpg	928.16	J/mol×K	1027.76	Joback Method
cpg	938.50	J/mol×K	1062.75	Joback Method
cpg	947.88	J/mol×K	1097.74	Joback Method
dvisc	0.0003892	Pa×s	535.78	Joback Method

dvisc	0.0002236	Pa×s	594.45	Joback Method
dvisc	0.0001419	Pa×s	653.12	Joback Method
dvisc	0.0000971	Pa×s	711.79	Joback Method
dvisc	0.0000704	Pa×s	770.47	Joback Method
dvisc	0.0000534	Pa×s	829.14	Joback Method
dvisc	0.0000420	Pa×s	887.81	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=U391100&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