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

Inchi: InChI=1S/C16H19ClO4/c1-3-4-5-10-20-15(18)8-9-16(19)21-13-6-7-14(17)12(2)11-13/h3,

InchiKey: DOOVWLPCEAOMLM-UHFFFAOYSA-N

Formula: C16H19ClO4

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

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-214.94	kJ/mol	Joback Method
hf	-539.89	kJ/mol	Joback Method
hfus	38.95	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.843		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	788.81	K	Joback Method
tc	997.82	K	Joback Method
tf	494.02	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.28	J/mol×K	788.81	Joback Method
cpg	661.67	J/mol×K	823.65	Joback Method
cpg	674.09	J/mol×K	858.48	Joback Method
cpg	685.56	J/mol×K	893.32	Joback Method
cpg	696.11	J/mol×K	928.15	Joback Method
cpg	705.74	J/mol×K	962.99	Joback Method
cpg	714.46	J/mol×K	997.82	Joback Method
dvisc	0.0006299	Pa×s	494.02	Joback Method

dvisc	0.0003920	Pa×s	543.15	Joback Method
dvisc	0.0002639	Pa×s	592.28	Joback Method
dvisc	0.0001888	Pa×s	641.41	Joback Method
dvisc	0.0001416	Pa×s	690.55	Joback Method
dvisc	0.0001104	Pa×s	739.68	Joback Method
dvisc	0.0000887	Pa×s	788.81	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=U391073&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