Succinic acid, 4-chloro-3-methylphenyl cis-pent-2-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/h4-

InchiKey: YMGZXRWSYSRUAB-PLNGDYQASA-N

Formula: C16H19ClO4

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

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-222.56	kJ/mol	Joback Method
hf	-548.10	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	77.46	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.843		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	796.29	K	Joback Method
tc	1008.62	K	Joback Method
tf	490.70	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.45	J/mol×K	796.29	Joback Method
cpg	661.84	J/mol×K	831.68	Joback Method
cpg	674.28	J/mol×K	867.07	Joback Method
cpg	685.80	J/mol×K	902.46	Joback Method
cpg	696.40	J/mol×K	937.85	Joback Method
cpg	706.13	J/mol×K	973.23	Joback Method
cpg	714.98	J/mol×K	1008.62	Joback Method
dvisc	0.0005682	Pa×s	490.70	Joback Method

dvisc	0.0003431	Pa×s	541.63	Joback Method
dvisc	0.0002260	Pa×s	592.56	Joback Method
dvisc	0.0001590	Pa×s	643.50	Joback Method
dvisc	0.0001178	Pa×s	694.43	Joback Method
dvisc	0.0000909	Pa×s	745.36	Joback Method
dvisc	0.0000725	Pa×s	796.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U391267&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

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