Succinic acid, 3-chlorophenyl cis-pent-2-en-1-yl ester

Inchi: InChI=1S/C15H17ClO4/c1-2-3-4-10-19-14(17)8-9-15(18)20-13-7-5-6-12(16)11-13/h3-7,1

InchiKey: WKUXPMQDZQZCTR-ARJAWSKDSA-N

Formula: C15H17ClO4

SMILES: CCC=CCOC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-221.35	kJ/mol	Joback Method
hf	-515.99	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	74.58	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.535		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	768.43	K	Joback Method
tc	982.15	K	Joback Method
tf	466.91	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.97	J/mol×K	768.43	Joback Method
cpg	608.10	J/mol×K	804.05	Joback Method
cpg	620.30	J/mol×K	839.67	Joback Method
cpg	631.59	J/mol×K	875.29	Joback Method
cpg	642.00	J/mol×K	910.91	Joback Method
cpg	651.56	J/mol×K	946.53	Joback Method
cpg	660.29	J/mol×K	982.15	Joback Method
dvisc	0.0007224	Pa×s	466.91	Joback Method

dvisc	0.0004215	Pa×s	517.16	Joback Method
dvisc	0.0002705	Pa×s	567.42	Joback Method
dvisc	0.0001866	Pa×s	617.67	Joback Method
dvisc	0.0001362	Pa×s	667.92	Joback Method
dvisc	0.0001038	Pa×s	718.18	Joback Method
dvisc	0.0000820	Pa×s	768.43	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=U391265&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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