

Succinic acid, 3-chlorophenyl pent-4-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/h2,5-7
InchiKey:	PYWMWUXLGGGAQY-UHFFFAOYSA-N
Formula:	C15H17ClO4
SMILES:	C=CCCCOC(=O)CCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	296.75

Physical Properties

Property code	Value	Unit	Source
gf	-213.73	kJ/mol	Joback Method
hf	-507.78	kJ/mol	Joback Method
hfus	36.75	kJ/mol	Joback Method
hvap	73.95	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.535		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	2131.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	760.95	K	Joback Method
tc	971.13	K	Joback Method
tf	470.23	K	Joback Method
vc	0.846	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.87	J/molxK	760.95	Joback Method
cpg	608.00	J/molxK	795.98	Joback Method
cpg	620.19	J/molxK	831.01	Joback Method
cpg	631.47	J/molxK	866.04	Joback Method
cpg	641.84	J/molxK	901.07	Joback Method
cpg	651.33	J/molxK	936.10	Joback Method
cpg	659.96	J/molxK	971.13	Joback Method
dvisc	0.0007951	Paxs	470.23	Joback Method

dvisc	0.0004793	Paxs	518.68	Joback Method
dvisc	0.0003150	Paxs	567.14	Joback Method
dvisc	0.0002212	Paxs	615.59	Joback Method
dvisc	0.0001635	Paxs	664.04	Joback Method
dvisc	0.0001260	Paxs	712.50	Joback Method
dvisc	0.0001003	Paxs	760.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U391071&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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