

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:	<chem>C=CCCCOC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1</chem>
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003920	Paxs	543.15	Joback Method
dvisc	0.0002639	Paxs	592.28	Joback Method
dvisc	0.0001888	Paxs	641.41	Joback Method
dvisc	0.0001416	Paxs	690.55	Joback Method
dvisc	0.0001104	Paxs	739.68	Joback Method
dvisc	0.0000887	Paxs	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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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