

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

Inchi:	InChI=1S/C17H21ClO4/c1-3-4-5-6-11-21-16(19)9-10-17(20)22-14-7-8-15(18)13(2)12-14
InchiKey:	HGUUDYHGMKNGPV-PLNGDYQASA-N
Formula:	C17H21ClO4
SMILES:	CCC=CCCOC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	324.80

Physical Properties

Property code	Value	Unit	Source
gf	-214.14	kJ/mol	Joback Method
hf	-568.74	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.234		Crippen Method
mvol	249.450	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	819.17	K	Joback Method
tc	1029.92	K	Joback Method
tf	501.97	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.17	J/molxK	819.17	Joback Method
cpg	717.87	J/molxK	854.29	Joback Method
cpg	730.59	J/molxK	889.42	Joback Method
cpg	742.35	J/molxK	924.54	Joback Method
cpg	753.18	J/molxK	959.67	Joback Method
cpg	763.10	J/molxK	994.79	Joback Method
cpg	772.14	J/molxK	1029.92	Joback Method
dvisc	0.0005205	Paxs	501.97	Joback Method

dvisc	0.0003102	Paxs	554.84	Joback Method
dvisc	0.0002023	Paxs	607.70	Joback Method
dvisc	0.0001413	Paxs	660.57	Joback Method
dvisc	0.0001041	Paxs	713.44	Joback Method
dvisc	0.0000799	Paxs	766.30	Joback Method
dvisc	0.0000635	Paxs	819.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391089&Units=SI
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

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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