

Succinic acid, 3-chlorophenyl hex-5-en-1-yl ester

Inchi:	InChI=1S/C16H19ClO4/c1-2-3-4-5-11-20-15(18)9-10-16(19)21-14-8-6-7-13(17)12-14/h2,
InchiKey:	SDCSWBKWDCOCCA-UHFFFAOYSA-N
Formula:	C16H19ClO4
SMILES:	C=CCCCOC(=O)CCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	310.77

Physical Properties

Property code	Value	Unit	Source
gf	-205.31	kJ/mol	Joback Method
hf	-528.42	kJ/mol	Joback Method
hfus	39.34	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.925		Crippen Method
mvol	235.360	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	783.83	K	Joback Method
tc	992.06	K	Joback Method
tf	481.50	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.42	J/molxK	783.83	Joback Method
cpg	707.29	J/molxK	957.35	Joback Method
cpg	697.57	J/molxK	922.65	Joback Method
cpg	686.95	J/molxK	887.94	Joback Method
cpg	675.39	J/molxK	853.24	Joback Method
cpg	662.89	J/molxK	818.53	Joback Method
cpg	716.12	J/molxK	992.06	Joback Method
dvisc	0.0000881	Paxs	783.83	Joback Method

dvisc	0.0001110	Paxs	733.44	Joback Method
dvisc	0.0001448	Paxs	683.05	Joback Method
dvisc	0.0001970	Paxs	632.66	Joback Method
dvisc	0.0002828	Paxs	582.28	Joback Method
dvisc	0.0004347	Paxs	531.89	Joback Method
dvisc	0.0007310	Paxs	481.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391287&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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