

Succinic acid, dodec-2-en-1-yl 2-chlorophenyl ester

Inchi:	InChI=1S/C22H31ClO4/c1-2-3-4-5-6-7-8-9-10-13-18-26-21(24)16-17-22(25)27-20-15-12
InchiKey:	STGWJHFKMBBOSL-JLHYYAGUSA-N
Formula:	C22H31ClO4
SMILES:	CCCCCCCCC=CCOC(=O)CCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	394.93

Physical Properties

Property code	Value	Unit	Source
gf	-162.41	kJ/mol	Joback Method
hf	-660.47	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	90.16	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.266		Crippen Method
mvol	319.900	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	928.59	K	Joback Method
tc	1140.81	K	Joback Method
tf	545.80	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.34	J/molxK	928.59	Joback Method
cpg	1011.37	J/molxK	963.96	Joback Method
cpg	1025.24	J/molxK	999.33	Joback Method
cpg	1038.00	J/molxK	1034.70	Joback Method
cpg	1049.70	J/molxK	1070.07	Joback Method
cpg	1060.39	J/molxK	1105.44	Joback Method
cpg	1070.12	J/molxK	1140.81	Joback Method
dvisc	0.0003584	Paxs	545.80	Joback Method

dvisc	0.0001922	Paxs	609.60	Joback Method
dvisc	0.0001160	Paxs	673.40	Joback Method
dvisc	0.0000764	Paxs	737.19	Joback Method
dvisc	0.0000538	Paxs	800.99	Joback Method
dvisc	0.0000399	Paxs	864.79	Joback Method
dvisc	0.0000308	Paxs	928.59	Joback Method

Sources

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=U389805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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