Succinic acid, dodec-2-en-1-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C23H33ClO5/c1-3-4-5-6-7-8-9-10-11-12-17-28-22(25)15-16-23(26)29-20-14-13

InchiKey: XAGALQCDZFKKAF-VAWYXSNFSA-N

Formula: C23H33ClO5

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 424.96

Physical Properties

Property code	Value	Unit	Source
gf	-268.62	kJ/mol	Joback Method
hf	-824.80	kJ/mol	Joback Method
hfus	59.75	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.274		Crippen Method
mcvol	339.860	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	3084.00		NIST Webbook
rinpol	3084.00		NIST Webbook
tb	978.87	K	Joback Method
tc	1198.80	K	Joback Method
tf	591.82	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.03	J/mol×K	978.87	Joback Method
cpg	1098.50	J/mol×K	1015.52	Joback Method
cpg	1111.58	J/mol×K	1052.18	Joback Method
cpg	1123.31	J/mol×K	1088.83	Joback Method
cpg	1133.72	J/mol×K	1125.49	Joback Method
cpg	1142.83	J/mol×K	1162.14	Joback Method
cpg	1150.69	J/mol×K	1198.80	Joback Method
dvisc	0.0001963	Pa×s	591.82	Joback Method

dvisc	0.0001114	Pa×s	656.33	Joback Method
dvisc	0.0000699	Pa×s	720.84	Joback Method
dvisc	0.0000474	Pa×s	785.34	Joback Method
dvisc	0.0000341	Pa×s	849.85	Joback Method
dvisc	0.0000257	Pa×s	914.36	Joback Method
dvisc	0.0000201	Pa×s	978.87	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=U390946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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