Succinic acid, 3-chlorophenyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C18H21ClO4/c1-13-5-2-3-6-14(13)12-22-17(20)9-10-18(21)23-16-8-4-7-15(19)

InchiKey: WTZOLTGMYXRHAC-UHFFFAOYSA-N

Formula: C18H21ClO4

SMILES: CC1=C(COC(=O)CCC(=O)Oc2cccc(Cl)c2)CCCC1

Mol. weight [g/mol]: 336.81

Physical Properties

Property code	Value	Unit	Source
gf	-233.45	kJ/mol	Joback Method
hf	-585.63	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	83.65	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.459		Crippen Method
mcvol	252.680	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2634.00		NIST Webbook
tb	866.25	K	Joback Method
tc	1095.56	K	Joback Method
tf	543.22	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.34	J/mol×K	866.25	Joback Method
cpg	761.41	J/mol×K	904.47	Joback Method
cpg	774.13	J/mol×K	942.69	Joback Method
cpg	785.53	J/mol×K	980.90	Joback Method
cpg	795.64	J/mol×K	1019.12	Joback Method
cpg	804.48	J/mol×K	1057.34	Joback Method
cpg	812.08	J/mol×K	1095.56	Joback Method
dvisc	0.0004589	Pa×s	543.22	Joback Method
dvisc	0.0002757	Pa×s	597.06	Joback Method

dvisc	0.0001802	Pa×s	650.90	Joback Method
dvisc	0.0001257	Pa×s	704.73	Joback Method
dvisc	0.0000923	Pa×s	758.57	Joback Method
dvisc	0.0000706	Pa×s	812.41	Joback Method
dvisc	0.0000558	Pa×s	866.25	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=U391421&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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