Succinic acid, 4-chloro-3-methylphenyl 1-cyclopentylethyl ester

Inchi: InChI=1S/C18H23ClO4/c1-12-11-15(7-8-16(12)19)23-18(21)10-9-17(20)22-13(2)14-5-3-4

InchiKey: YCCUDPQBDQGXKL-UHFFFAOYSA-N

Formula: C18H23ClO4

SMILES: Cc1cc(OC(=O)CCC(=O)OC(C)C2CCCC2)ccc1Cl

Mol. weight [g/mol]: 338.83

Physical Properties

Property code	Value	Unit	Source
gf	-251.83	kJ/mol	Joback Method
hf	-651.40	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	81.83	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.456		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	852.73	K	Joback Method
tc	1077.89	K	Joback Method
tf	514.22	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.26	J/mol×K	852.73	Joback Method
cpg	793.52	J/mol×K	890.26	Joback Method
cpg	807.42	J/mol×K	927.78	Joback Method
cpg	820.01	J/mol×K	965.31	Joback Method
cpg	831.31	J/mol×K	1002.84	Joback Method
cpg	841.35	J/mol×K	1040.36	Joback Method
cpg	850.17	J/mol×K	1077.89	Joback Method
dvisc	0.0007531	Pa×s	514.22	Joback Method

dvisc	0.0004402	Pa×s	570.64	Joback Method
dvisc	0.0002834	Pa×s	627.06	Joback Method
dvisc	0.0001962	Pa×s	683.48	Joback Method
dvisc	0.0001437	Pa×s	739.89	Joback Method
dvisc	0.0001100	Pa×s	796.31	Joback Method
dvisc	0.0000872	Pa×s	852.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U391414&Units=SI

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