Succinic acid, dec-2-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C21H31ClO5/c1-4-5-6-7-8-9-10-16(2)26-20(23)13-14-21(24)27-18-12-11-17(22

InchiKey: QGDBHFJCLWWOKX-UHFFFAOYSA-N

Formula: C21H31ClO5

SMILES: CCCCCCCCC(C)OC(=O)CCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 398.92

Physical Properties

Property code	Value	Unit	Source
gf	-368.12	kJ/mol	Joback Method
hf	-906.02	kJ/mol	Joback Method
hfus	50.84	kJ/mol	Joback Method
hvap	90.66	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.716		Crippen Method
mcvol	315.980	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2753.00		NIST Webbook
rinpol	2753.00		NIST Webbook
tb	928.51	K	Joback Method
tc	1140.15	K	Joback Method
tf	559.36	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.54	J/mol×K	928.51	Joback Method
cpg	1051.36	J/mol×K	1104.88	Joback Method
cpg	1042.30	J/mol×K	1069.60	Joback Method
cpg	1031.90	J/mol×K	1034.33	Joback Method
cpg	1020.15	J/mol×K	999.06	Joback Method
cpg	1007.03	J/mol×K	963.78	Joback Method
cpg	1059.09	J/mol×K	1140.15	Joback Method
dvisc	0.0000282	Pa×s	928.51	Joback Method

dvisc	0.0000362	Pa×s	866.98	Joback Method
dvisc	0.0000484	Pa×s	805.46	Joback Method
dvisc	0.0000678	Pa×s	743.93	Joback Method
dvisc	0.0001010	Pa×s	682.41	Joback Method
dvisc	0.0001628	Pa×s	620.88	Joback Method
dvisc	0.0002914	Pa×s	559.36	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=U390943&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