Succinic acid, 2-methylpent-3-yl 4-chloro-2-formylphenyl ester

Inchi: InChI=1S/C17H21ClO5/c1-4-14(11(2)3)22-16(20)7-8-17(21)23-15-6-5-13(18)9-12(15)10-

InchiKey: VMDZVBBEWVWINT-UHFFFAOYSA-N

Formula: C17H21ClO5

SMILES: CCC(OC(=O)CCC(=O)Oc1ccc(Cl)cc1C=O)C(C)C

Mol. weight [g/mol]: 340.80

Physical Properties

Property code	Value	Unit	Source
gf	-398.76	kJ/mol	Joback Method
hf	-782.10	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	85.68	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.816		Crippen Method
mcvol	255.320	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	862.79	K	Joback Method
tc	1076.96	K	Joback Method
tf	519.05	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.59	J/mol×K	862.79	Joback Method
cpg	757.18	J/mol×K	898.49	Joback Method
cpg	768.65	J/mol×K	934.18	Joback Method
cpg	779.03	J/mol×K	969.88	Joback Method
cpg	788.31	J/mol×K	1005.57	Joback Method
cpg	796.52	J/mol×K	1041.27	Joback Method
cpg	803.66	J/mol×K	1076.96	Joback Method
dvisc	0.0006723	Pa×s	519.05	Joback Method

dvisc	0.0003772	Pa×s	576.34	Joback Method
dvisc	0.0002349	Pa×s	633.63	Joback Method
dvisc	0.0001583	Pa×s	690.92	Joback Method
dvisc	0.0001133	Pa×s	748.21	Joback Method
dvisc	0.0000850	Pa×s	805.50	Joback Method
dvisc	0.0000663	Pa×s	862.79	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=U389917&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