Succinic acid, 3-chlorophenyl 2-methylbutyl ester

Inchi: InChI=1S/C15H19ClO4/c1-3-11(2)10-19-14(17)7-8-15(18)20-13-6-4-5-12(16)9-13/h4-6,9

InchiKey: CSDSURCFYLQZPI-UHFFFAOYSA-N

Formula: C15H19ClO4

SMILES: CCC(C)COC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 298.76

Physical Properties

Property code	Value	Unit	Source
gf	-304.01	kJ/mol	Joback Method
hf	-638.49	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.615		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
tb	763.83	K	Joback Method
tc	974.13	K	Joback Method
tf	456.99	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.63	J/mol×K	763.83	Joback Method
cpg	634.52	J/mol×K	798.88	Joback Method
cpg	647.43	J/mol×K	833.93	Joback Method
cpg	659.36	J/mol×K	868.98	Joback Method
cpg	670.31	J/mol×K	904.03	Joback Method
cpg	680.32	J/mol×K	939.08	Joback Method
cpg	689.38	J/mol×K	974.13	Joback Method
dvisc	0.0008947	Pa×s	456.99	Joback Method

dvisc	0.0004991	Pa×s	508.13	Joback Method
dvisc	0.0003097	Pa×s	559.27	Joback Method
dvisc	0.0002082	Pa×s	610.41	Joback Method
dvisc	0.0001489	Pa×s	661.55	Joback Method
dvisc	0.0001117	Pa×s	712.69	Joback Method
dvisc	0.0000870	Pa×s	763.83	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=U389634&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