Succinic acid, 3-methylbut-2-yl 3-chlorophenyl ester

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

InchiKey: FPHQZMVPNJVQDI-UHFFFAOYSA-N

Formula: C15H19ClO4

SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 298.76

Physical Properties

Property code	Value	Unit	Source
gf	-306.45	kJ/mol	Joback Method
hf	-643.77	kJ/mol	Joback Method
hfus	30.98	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.613		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	763.39	K	Joback Method
tc	976.92	K	Joback Method
tf	441.99	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.20	J/mol×K	763.39	Joback Method
cpg	681.57	J/mol×K	941.33	Joback Method
cpg	671.51	J/mol×K	905.74	Joback Method
cpg	660.46	J/mol×K	870.16	Joback Method
cpg	648.39	J/mol×K	834.57	Joback Method
cpg	635.31	J/mol×K	798.98	Joback Method
cpg	690.64	J/mol×K	976.92	Joback Method
dvisc	0.0000802	Pa×s	763.39	Joback Method

dvisc	0.0001046	Pa×s	709.82	Joback Method
dvisc	0.0001424	Pa×s	656.26	Joback Method
dvisc	0.0002050	Pa×s	602.69	Joback Method
dvisc	0.0003168	Pa×s	549.12	Joback Method
dvisc	0.0005378	Pa×s	495.56	Joback Method
dvisc	0.0010379	Pa×s	441.99	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=U389849&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

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