Succinic acid, 3-chlorophenyl (2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C17H20Cl2O4/c18-13-5-3-6-14(10-13)23-17(21)9-8-16(20)22-11-12-4-1-2-7-15

InchiKey: GMIRTKNNDZWBBM-UHFFFAOYSA-N

Formula: C17H20Cl2O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCC1CCCCC1Cl

Mol. weight [g/mol]: 359.24

Physical Properties

Property code	Value	Unit	Source
gf	-279.92	kJ/mol	Joback Method
hf	-656.25	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	83.58	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.366		Crippen Method
mcvol	255.130	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	2742.00		NIST Webbook
rinpol	2742.00		NIST Webbook
tb	862.34	K	Joback Method
tc	1094.19	K	Joback Method
tf	527.59	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.98	J/mol×K	862.34	Joback Method
cpg	768.27	J/mol×K	900.98	Joback Method
cpg	781.07	J/mol×K	939.62	Joback Method
cpg	792.39	J/mol×K	978.26	Joback Method
cpg	802.26	J/mol×K	1016.91	Joback Method
cpg	810.71	J/mol×K	1055.55	Joback Method
cpg	817.74	J/mol×K	1094.19	Joback Method
dvisc	0.0006832	Pa×s	527.59	Joback Method

dvisc	0.0004076	Pa×s	583.38	Joback Method
dvisc	0.0002661	Pa×s	639.17	Joback Method
dvisc	0.0001861	Pa×s	694.96	Joback Method
dvisc	0.0001372	Pa×s	750.76	Joback Method
dvisc	0.0001055	Pa×s	806.55	Joback Method
dvisc	0.0000840	Pa×s	862.34	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=U391403&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