Succinic acid, 3-chlorophenyl 4-chlorobenzyl ester

Inchi: InChI=1S/C17H14Cl2O4/c18-13-6-4-12(5-7-13)11-22-16(20)8-9-17(21)23-15-3-1-2-14(19

InchiKey: WLSVVFSVBLCPEQ-UHFFFAOYSA-N

Formula: C17H14Cl2O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 353.20

Physical Properties

Property code	Value	Unit	Source
gf	-193.88	kJ/mol	Joback Method
hf	-465.17	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	86.39	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.422		Crippen Method
mcvol	242.230	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	879.12	K	Joback Method
tc	1116.93	K	Joback Method
tf	563.39	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.24	J/mol×K	879.12	Joback Method
cpg	666.17	J/mol×K	918.76	Joback Method
cpg	675.88	J/mol×K	958.39	Joback Method
cpg	684.43	J/mol×K	998.03	Joback Method
cpg	691.83	J/mol×K	1037.66	Joback Method
cpg	698.12	J/mol×K	1077.30	Joback Method
cpg	703.34	J/mol×K	1116.93	Joback Method
dvisc	0.0004284	Pa×s	563.39	Joback Method

dvisc	0.0002737	Pa×s	616.01	Joback Method
dvisc	0.0001876	Pa×s	668.63	Joback Method
dvisc	0.0001359	Pa×s	721.25	Joback Method
dvisc	0.0001029	Pa×s	773.88	Joback Method
dvisc	0.0000807	Pa×s	826.50	Joback Method
dvisc	0.0000651	Pa×s	879.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389679&Units=SI
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

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