Succinic acid, 2,3-dichlorophenyl cyclopentyl ester

Inchi: InChI=1S/C15H16Cl2O4/c16-11-6-3-7-12(15(11)17)21-14(19)9-8-13(18)20-10-4-1-2-5-10

InchiKey: ZPKSZRJFPDGABF-UHFFFAOYSA-N

Formula: C15H16Cl2O4

SMILES: O=C(CCC(=O)OC1CCCC1)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-286.58	kJ/mol	Joback Method
hf	-599.94	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	79.92	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.165		Crippen Method
mcvol	226.950	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	2461.00		NIST Webbook
rinpol	2461.00		NIST Webbook
tb	821.96	K	Joback Method
tc	1055.13	K	Joback Method
tf	525.33	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.56	J/mol×K	821.96	Joback Method
cpg	645.85	J/mol×K	860.82	Joback Method
cpg	657.90	J/mol×K	899.68	Joback Method
cpg	668.74	J/mol×K	938.54	Joback Method
cpg	678.39	J/mol×K	977.40	Joback Method
cpg	686.88	J/mol×K	1016.27	Joback Method
cpg	694.23	J/mol×K	1055.13	Joback Method
dvisc	0.0007650	Pa×s	525.33	Joback Method

dvisc	0.0004962	Pa×s	574.77	Joback Method
dvisc	0.0003447	Pa×s	624.21	Joback Method
dvisc	0.0002526	Pa×s	673.64	Joback Method
dvisc	0.0001932	Pa×s	723.08	Joback Method
dvisc	0.0001529	Pa×s	772.52	Joback Method
dvisc	0.0001244	Pa×s	821.96	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=U391382&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