Succinic acid, 2,3-dichlorophenyl but-3-en-1-yl ester

Inchi: InChI=1S/C14H14Cl2O4/c1-2-3-9-19-12(17)7-8-13(18)20-11-6-4-5-10(15)14(11)16/h2,4-

InchiKey: WMVFZNMVGKKIPZ-UHFFFAOYSA-N

Formula: C14H14Cl2O4

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

Mol. weight [g/mol]: 317.17

Physical Properties

Property code	Value	Unit	Source
gf	-243.71	kJ/mol	Joback Method
hf	-514.35	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	76.77	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.798		Crippen Method
mcvol	219.420	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook
tb	780.48	K	Joback Method
tc	997.13	K	Joback Method
tf	501.40	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.46	J/mol×K	780.48	Joback Method
cpg	575.01	J/mol×K	816.59	Joback Method
cpg	585.67	J/mol×K	852.70	Joback Method
cpg	595.44	J/mol×K	888.80	Joback Method
cpg	604.33	J/mol×K	924.91	Joback Method
cpg	612.36	J/mol×K	961.02	Joback Method
cpg	619.53	J/mol×K	997.13	Joback Method
dvisc	0.0006383	Pa×s	501.40	Joback Method

dvisc	0.0004128	Pa×s	547.91	Joback Method
dvisc	0.0002859	Pa×s	594.43	Joback Method
dvisc	0.0002088	Pa×s	640.94	Joback Method
dvisc	0.0001591	Pa×s	687.45	Joback Method
dvisc	0.0001255	Pa×s	733.97	Joback Method
dvisc	0.0001018	Pa×s	780.48	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=U391200&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