Succinic acid, 2,4,6-trichlorophenyl but-3-en-1-yl ester

Inchi: InChI=1S/C14H13Cl3O4/c1-2-3-6-20-12(18)4-5-13(19)21-14-10(16)7-9(15)8-11(14)17/h2
InchiKey: PCOCZTIOEQNABH-UHFFFAOYSA-N
Formula: C14H13Cl3O4
SMILES: C=CCCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 351.61

Physical Properties

Property code	Value	Unit	Source
gf	-265.27	kJ/mol	Joback Method
hf	-541.56	kJ/mol	Joback Method
hfus	41.77	kJ/mol	Joback Method
hvap	81.82	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.452		Crippen Method
mcvol	231.660	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	822.89	K	Joback Method
tc	1043.51	K	Joback Method
tf	543.84	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.48	J/mol×K	822.89	Joback Method
cpg	593.87	J/mol×K	859.66	Joback Method
cpg	603.36	J/mol×K	896.43	Joback Method
cpg	611.95	J/mol×K	933.20	Joback Method
cpg	619.66	J/mol×K	969.97	Joback Method
cpg	626.48	J/mol×K	1006.74	Joback Method
cpg	632.43	J/mol×K	1043.51	Joback Method
dvisc	0.0004840	Pa×s	543.84	Joback Method

dvisc	0.0003276	Pa×s	590.35	Joback Method
dvisc	0.0002348	Pa×s	636.86	Joback Method
dvisc	0.0001761	Pa×s	683.37	Joback Method
dvisc	0.0001370	Pa×s	729.87	Joback Method
dvisc	0.0001098	Pa×s	776.38	Joback Method
dvisc	0.0000902	Pa×s	822.89	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=U391202&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