Succinic acid, 2,4,6-trichlorophenyl phenethyl ester

Inchi: InChI=1S/C18H15Cl3O4/c19-13-10-14(20)18(15(21)11-13)25-17(23)7-6-16(22)24-9-8-12
InchiKey: DCKNWSSVFSPDAW-UHFFFAOYSA-N
Formula: C18H15Cl3O4
SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCCc1ccccc1
Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	-207.02	kJ/mol	Joback Method
hf	-513.02	kJ/mol	Joback Method
hfus	47.46	kJ/mol	Joback Method
hvap	93.67	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.118		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	944.41	K	Joback Method
tc	1183.38	K	Joback Method
tf	617.10	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.53	J/mol×K	944.41	Joback Method
cpg	738.17	J/mol×K	984.24	Joback Method
cpg	746.58	J/mol×K	1024.07	Joback Method
cpg	753.80	J/mol×K	1063.89	Joback Method
cpg	759.85	J/mol×K	1103.72	Joback Method
cpg	764.77	J/mol×K	1143.55	Joback Method
cpg	768.58	J/mol×K	1183.38	Joback Method
dvisc	0.0002930	Pa×s	617.10	Joback Method

dvisc	0.0001931	Pa×s	671.65	Joback Method
dvisc	0.0001355	Pa×s	726.20	Joback Method
dvisc	0.0000999	Pa×s	780.76	Joback Method
dvisc	0.0000766	Pa×s	835.31	Joback Method
dvisc	0.0000607	Pa×s	889.86	Joback Method
dvisc	0.0000494	Pa×s	944.41	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=U389755&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