Succinic acid, 2,4,6-trichlorophenyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C16H19Cl3O4/c1-9(16(2,3)4)22-13(20)5-6-14(21)23-15-11(18)7-10(17)8-12(15

InchiKey: RFNWXBMGIQPPMV-UHFFFAOYSA-N

Formula: C16H19Cl3O4

SMILES: CC(OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)C(C)(C)C

Mol. weight [g/mol]: 381.68

Physical Properties

Property code	Value	Unit	Source
gf	-335.87	kJ/mol	Joback Method
hf	-722.30	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	85.25	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.310		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	868.30	K	Joback Method
tc	1093.36	K	Joback Method
tf	555.56	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.20	J/mol×K	868.30	Joback Method
cpg	734.00	J/mol×K	905.81	Joback Method
cpg	744.73	J/mol×K	943.32	Joback Method
cpg	754.43	J/mol×K	980.83	Joback Method
cpg	763.12	J/mol×K	1018.34	Joback Method
cpg	770.84	J/mol×K	1055.85	Joback Method
cpg	777.61	J/mol×K	1093.36	Joback Method
dvisc	0.0003702	Pa×s	555.56	Joback Method

dvisc	0.0002250	Pa×s	607.68	Joback Method
dvisc	0.0001479	Pa×s	659.81	Joback Method
dvisc	0.0001034	Pa×s	711.93	Joback Method
dvisc	0.0000759	Pa×s	764.05	Joback Method
dvisc	0.0000580	Pa×s	816.18	Joback Method
dvisc	0.0000457	Pa×s	868.30	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=U390633&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