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

Inchi: InChI=1S/C18H23Cl3O4/c1-11(9-18(2,3)4)10-24-15(22)5-6-16(23)25-17-13(20)7-12(19)8

InchiKey: KCYLYFNPPOGEIA-UHFFFAOYSA-N

Formula: C18H23Cl3O4

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

Mol. weight [g/mol]: 409.73

Physical Properties

Property code	Value	Unit	Source
gf	-319.03	kJ/mol	Joback Method
hf	-763.58	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	89.71	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.948		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2486.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tb	914.06	K	Joback Method
tc	1136.74	K	Joback Method
tf	578.10	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.58	J/mol×K	914.06	Joback Method
cpg	847.80	J/mol×K	951.17	Joback Method
cpg	858.90	J/mol×K	988.29	Joback Method
cpg	868.92	J/mol×K	1025.40	Joback Method
cpg	877.89	J/mol×K	1062.51	Joback Method
cpg	885.85	J/mol×K	1099.63	Joback Method
cpg	892.85	J/mol×K	1136.74	Joback Method
dvisc	0.0002948	Pa×s	578.10	Joback Method

dvisc	0.0001750	Pa×s	634.09	Joback Method
dvisc	0.0001131	Pa×s	690.09	Joback Method
dvisc	0.0000780	Pa×s	746.08	Joback Method
dvisc	0.0000567	Pa×s	802.07	Joback Method
dvisc	0.0000429	Pa×s	858.07	Joback Method
dvisc	0.0000336	Pa×s	914.06	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=U389550&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