Succinic acid, 2,3-dichlorophenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C18H24Cl2O4/c1-12(10-18(2,3)4)11-23-15(21)8-9-16(22)24-14-7-5-6-13(19)17

InchiKey: BGSKIJGIKVJWSC-UHFFFAOYSA-N

Formula: C18H24Cl2O4

SMILES: CC(COC(=O)CCC(=O)Oc1cccc(Cl)c1Cl)CC(C)(C)C

Mol. weight [g/mol]: 375.29

Physical Properties

Property code	Value	Unit	Source
gf	-297.47	kJ/mol	Joback Method
hf	-736.37	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	84.66	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.295		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	871.65	K	Joback Method
tc	1089.44	K	Joback Method
tf	535.66	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.03	J/mol×K	871.65	Joback Method
cpg	870.87	J/mol×K	1053.14	Joback Method
cpg	861.59	J/mol×K	1016.85	Joback Method
cpg	851.30	J/mol×K	980.55	Joback Method
cpg	839.98	J/mol×K	944.25	Joback Method
cpg	827.56	J/mol×K	907.95	Joback Method
cpg	879.19	J/mol×K	1089.44	Joback Method
dvisc	0.0000393	Pa×s	871.65	Joback Method

dvisc	0.0000510	Pa×s	815.65	Joback Method
dvisc	0.0000687	Pa×s	759.65	Joback Method
dvisc	0.0000969	Pa×s	703.65	Joback Method
dvisc	0.0001453	Pa×s	647.66	Joback Method
dvisc	0.0002352	Pa×s	591.66	Joback Method
dvisc	0.0004208	Pa×s	535.66	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=U389549&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