Succinic acid, 2,2-dichloroethyl cis-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C16H26Cl2O4/c1-16(2,3)11-4-6-12(7-5-11)22-15(20)9-8-14(19)21-10-13(17)18

InchiKey: CEQKWDHCYKDKFT-UHFFFAOYSA-N

Formula: C16H26Cl2O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCC(=O)OCC(Cl)Cl)CC1

Mol. weight [g/mol]: 353.28

Physical Properties

Property code	Value	Unit	Source
gf	-390.72	kJ/mol	Joback Method
hf	-874.70	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.262		Crippen Method
mcvol	264.800	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	804.13	K	Joback Method
tc	1018.60	K	Joback Method
tf	464.80	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.26	J/mol×K	804.13	Joback Method
cpg	864.96	J/mol×K	982.85	Joback Method
cpg	853.34	J/mol×K	947.11	Joback Method
cpg	840.50	J/mol×K	911.36	Joback Method
cpg	826.39	J/mol×K	875.62	Joback Method
cpg	810.99	J/mol×K	839.87	Joback Method
cpg	875.38	J/mol×K	1018.60	Joback Method
dvisc	0.0000684	Pa×s	804.13	Joback Method

dvisc	0.0000911	Pa×s	747.58	Joback Method
dvisc	0.0001273	Pa×s	691.02	Joback Method
dvisc	0.0001886	Pa×s	634.46	Joback Method
dvisc	0.0003020	Pa×s	577.91	Joback Method
dvisc	0.0005355	Pa×s	521.36	Joback Method
dvisc	0.0010914	Pa×s	464.80	Joback Method

Sources

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=U390188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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