

Succinic acid, 2,2-dichloroethyl trans-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
mvol	264.800	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		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/molxK	804.13	Joback Method
cpg	864.96	J/molxK	982.85	Joback Method
cpg	853.34	J/molxK	947.11	Joback Method
cpg	840.50	J/molxK	911.36	Joback Method
cpg	826.39	J/molxK	875.62	Joback Method
cpg	810.99	J/molxK	839.87	Joback Method
cpg	875.38	J/molxK	1018.60	Joback Method
dvisc	0.0000684	Paxs	804.13	Joback Method

dvisc	0.0000911	Paxs	747.58	Joback Method
dvisc	0.0001273	Paxs	691.02	Joback Method
dvisc	0.0001886	Paxs	634.46	Joback Method
dvisc	0.0003020	Paxs	577.91	Joback Method
dvisc	0.0005355	Paxs	521.36	Joback Method
dvisc	0.0010914	Paxs	464.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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