

Succinic acid, 2,4,6-trichlorophenyl cis-4-methylcyclohexyl ester

Inchi:	InChI=1S/C17H19Cl3O4/c1-10-2-4-12(5-3-10)23-15(21)6-7-16(22)24-17-13(19)8-11(18)9
InchiKey:	UVCNMCFHMNDXEK-UHFFFAOYSA-N
Formula:	C17H19Cl3O4
SMILES:	CC1CCC(OC(=O)CCC(=O)Oc2c(Cl)cc(Cl)cc2Cl)CC1
Mol. weight [g/mol]:	393.69

Physical Properties

Property code	Value	Unit	Source
gf	-311.11	kJ/mol	Joback Method
hf	-694.93	kJ/mol	Joback Method
hfus	43.73	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.454		Crippen Method
mvol	267.370	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2683.00		NIST Webbook
rinpol	2683.00		NIST Webbook
tb	909.73	K	Joback Method
tc	1145.97	K	Joback Method
tf	582.55	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.10	J/molxK	909.73	Joback Method
cpg	786.52	J/molxK	949.10	Joback Method
cpg	797.41	J/molxK	988.48	Joback Method
cpg	806.78	J/molxK	1027.85	Joback Method
cpg	814.63	J/molxK	1067.22	Joback Method
cpg	820.98	J/molxK	1106.59	Joback Method
cpg	825.83	J/molxK	1145.97	Joback Method
dvisc	0.0004553	Paxs	582.55	Joback Method

dvisc	0.0002965	Paxs	637.08	Joback Method
dvisc	0.0002067	Paxs	691.61	Joback Method
dvisc	0.0001518	Paxs	746.14	Joback Method
dvisc	0.0001163	Paxs	800.67	Joback Method
dvisc	0.0000922	Paxs	855.20	Joback Method
dvisc	0.0000752	Paxs	909.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390061&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

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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