

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

Inchi:	InChI=1S/C14H15Cl3O5/c1-2-20-5-6-21-12(18)3-4-13(19)22-14-10(16)7-9(15)8-11(14)1
InchiKey:	YHRBDRDWMJCTJP-UHFFFAOYSA-N
Formula:	C14H15Cl3O5
SMILES:	CCOCCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	369.62

Physical Properties

Property code	Value	Unit	Source
gf	-458.11	kJ/mol	Joback Method
hf	-799.21	kJ/mol	Joback Method
hfus	44.24	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.912		Crippen Method
mvol	241.830	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	848.63	K	Joback Method
tc	1065.41	K	Joback Method
tf	567.83	K	Joback Method
vc	0.924	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.00	J/molxK	848.63	Joback Method
cpg	645.54	J/molxK	884.76	Joback Method
cpg	655.07	J/molxK	920.89	Joback Method
cpg	663.56	J/molxK	957.02	Joback Method
cpg	671.01	J/molxK	993.15	Joback Method
cpg	677.40	J/molxK	1029.28	Joback Method
cpg	682.72	J/molxK	1065.41	Joback Method
dvisc	0.0003402	Paxs	567.83	Joback Method

dvisc	0.0002312	Paxs	614.63	Joback Method
dvisc	0.0001659	Paxs	661.43	Joback Method
dvisc	0.0001244	Paxs	708.23	Joback Method
dvisc	0.0000967	Paxs	755.03	Joback Method
dvisc	0.0000774	Paxs	801.83	Joback Method
dvisc	0.0000635	Paxs	848.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390673&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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