

Succinic acid, dec-2-yl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C16H27Cl3O4/c1-3-4-5-6-7-8-9-13(2)23-15(21)11-10-14(20)22-12-16(17,18)19
InchiKey:	DTQHJDIRQDHXPF-UHFFFAOYSA-N
Formula:	C16H27Cl3O4
SMILES:	CCCCCCCCC(C)OC(=O)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	389.74

Physical Properties

Property code	Value	Unit	Source
gf	-419.39	kJ/mol	Joback Method
hf	-924.42	kJ/mol	Joback Method
hfus	44.42	kJ/mol	Joback Method
hvap	80.99	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.362		Crippen Method
mcvol	287.900	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2269.00		NIST Webbook
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tb	826.68	K	Joback Method
tc	1024.91	K	Joback Method
tf	491.58	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.25	J/molxK	826.68	Joback Method
cpg	884.21	J/molxK	991.87	Joback Method
cpg	873.79	J/molxK	958.84	Joback Method
cpg	862.52	J/molxK	925.80	Joback Method
cpg	850.36	J/molxK	892.76	Joback Method
cpg	837.28	J/molxK	859.72	Joback Method
cpg	893.80	J/molxK	1024.91	Joback Method
dvisc	0.0000437	Paxs	826.68	Joback Method

dvisc	0.0000587	Paxs	770.83	Joback Method
dvisc	0.0000823	Paxs	714.98	Joback Method
dvisc	0.0001224	Paxs	659.13	Joback Method
dvisc	0.0001958	Paxs	603.28	Joback Method
dvisc	0.0003448	Paxs	547.43	Joback Method
dvisc	0.0006905	Paxs	491.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390240&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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