

Succinic acid, 2,2-dichloroethyl oct-1-en-3-yl ester

Inchi:	InChI=1S/C14H22Cl2O4/c1-3-5-6-7-11(4-2)20-14(18)9-8-13(17)19-10-12(15)16/h4,11-12
InchiKey:	KEWRQIXJKHWSRH-UHFFFAOYSA-N
Formula:	C14H22Cl2O4
SMILES:	C=CC(CCCCC)OC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	325.23

Physical Properties

Property code	Value	Unit	Source
gf	-341.74	kJ/mol	Joback Method
hf	-738.50	kJ/mol	Joback Method
hfus	37.66	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.792		Crippen Method
mcvol	243.180	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpola	2005.00		NIST Webbook
rinpola	2005.00		NIST Webbook
tb	742.96	K	Joback Method
tc	934.83	K	Joback Method
tf	419.94	K	Joback Method
vc	0.934	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.49	J/molxK	742.96	Joback Method
cpg	671.29	J/molxK	774.94	Joback Method
cpg	684.27	J/molxK	806.92	Joback Method
cpg	696.43	J/molxK	838.90	Joback Method
cpg	707.79	J/molxK	870.87	Joback Method
cpg	718.36	J/molxK	902.85	Joback Method
cpg	728.15	J/molxK	934.83	Joback Method
dvisc	0.0014113	Paxs	419.94	Joback Method

dvisc	0.0006763	Paxs	473.78	Joback Method
dvisc	0.0003766	Paxs	527.61	Joback Method
dvisc	0.0002337	Paxs	581.45	Joback Method
dvisc	0.0001573	Paxs	635.29	Joback Method
dvisc	0.0001126	Paxs	689.12	Joback Method
dvisc	0.0000846	Paxs	742.96	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=U391319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

Latest version available from:

<https://www.chemeo.com/cid/115-740-2/Succinic-acid-2-2-dichloroethyl-oct-1-en-3-yl-ester.pdf>

Generated by Cheméo on 2024-04-28 18:22:26.842218116 +0000 UTC m=+16617795.762795432.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.