

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

Inchi:	InChI=1S/C20H34Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-25-19(23)14-15-20(24)26-17
InchiKey:	XSAPMBSWKUPRNS-VAWYXSNFSA-N
Formula:	C20H34Cl2O4
SMILES:	CCCCCCCCC=CCCOC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	409.39

Physical Properties

Property code	Value	Unit	Source
gf	-296.40	kJ/mol	Joback Method
hf	-865.27	kJ/mol	Joback Method
hfus	58.20	kJ/mol	Joback Method
hvap	86.77	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.134		Crippen Method
mvol	327.720	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	2748.00		NIST Webbook
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tb	888.16	K	Joback Method
tc	1088.64	K	Joback Method
tf	499.24	K	Joback Method
vc	1.276	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.57	J/molxK	888.16	Joback Method
cpg	1019.48	J/molxK	921.57	Joback Method
cpg	1034.32	J/molxK	954.99	Joback Method
cpg	1048.13	J/molxK	988.40	Joback Method
cpg	1060.93	J/molxK	1021.81	Joback Method
cpg	1072.78	J/molxK	1055.22	Joback Method
cpg	1083.71	J/molxK	1088.64	Joback Method
dvisc	0.0005500	Paxs	499.24	Joback Method

dvisc	0.0002581	Paxs	564.06	Joback Method
dvisc	0.0001416	Paxs	628.88	Joback Method
dvisc	0.0000869	Paxs	693.70	Joback Method
dvisc	0.0000579	Paxs	758.52	Joback Method
dvisc	0.0000412	Paxs	823.34	Joback Method
dvisc	0.0000308	Paxs	888.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391055&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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