

Succinic acid, dodec-2-en-1-yl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C18H29Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-14-24-16(22)12-13-17(23)25-15-18(19)
InchiKey:	VAYVMAHAJQUVLC-ZHACJKMWSA-N
Formula:	C18H29Cl3O4
SMILES:	CCCCCCCCC=CCOC(=O)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	415.78

Physical Properties

Property code	Value	Unit	Source
gf	-319.89	kJ/mol	Joback Method
hf	-843.20	kJ/mol	Joback Method
hfus	53.33	kJ/mol	Joback Method
hvap	85.79	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.920		Crippen Method
mvol	311.780	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	877.04	K	Joback Method
tc	1079.86	K	Joback Method
tf	524.04	K	Joback Method
vc	1.208	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.61	J/molxK	877.04	Joback Method
cpg	925.74	J/molxK	910.84	Joback Method
cpg	938.95	J/molxK	944.65	Joback Method
cpg	951.28	J/molxK	978.45	Joback Method
cpg	962.78	J/molxK	1012.25	Joback Method
cpg	973.50	J/molxK	1046.05	Joback Method
cpg	983.50	J/molxK	1079.86	Joback Method
dvisc	0.0004337	Paxs	524.04	Joback Method

dvisc	0.0002222	Paxs	582.87	Joback Method
dvisc	0.0001287	Paxs	641.71	Joback Method
dvisc	0.0000817	Paxs	700.54	Joback Method
dvisc	0.0000556	Paxs	759.37	Joback Method
dvisc	0.0000400	Paxs	818.21	Joback Method
dvisc	0.0000301	Paxs	877.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390245&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

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

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