

Succinic acid, dodec-2-en-1-yl but-3-en-1-yl ester

Inchi:	InChI=1S/C20H34O4/c1-3-5-7-8-9-10-11-12-13-14-18-24-20(22)16-15-19(21)23-17-6-4-2
InchiKey:	AJSUOTAOMMWMPR-BUHFOSPRSA-N
Formula:	C20H34O4
SMILES:	C=CCCOC(=O)CCC(=O)OCC=CCCCCCCCC
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-182.26	kJ/mol	Joback Method
hf	-703.08	kJ/mol	Joback Method
hfus	52.05	kJ/mol	Joback Method
hvap	77.71	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.126		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2366.00		NIST Webbook
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tb	810.42	K	Joback Method
tc	997.04	K	Joback Method
tf	452.64	K	Joback Method
vc	1.165	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.92	J/molxK	810.42	Joback Method
cpg	993.31	J/molxK	965.94	Joback Method
cpg	979.84	J/molxK	934.83	Joback Method
cpg	965.49	J/molxK	903.73	Joback Method
cpg	950.25	J/molxK	872.63	Joback Method
cpg	934.06	J/molxK	841.52	Joback Method
cpg	1005.94	J/molxK	997.04	Joback Method
dvisc	0.0000494	Paxs	810.42	Joback Method

dvisc	0.0000653	Paxs	750.79	Joback Method
dvisc	0.0000905	Paxs	691.16	Joback Method
dvisc	0.0001335	Paxs	631.53	Joback Method
dvisc	0.0002134	Paxs	571.90	Joback Method
dvisc	0.0003805	Paxs	512.27	Joback Method
dvisc	0.0007901	Paxs	452.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391203&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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	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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