Succinic acid, dodec-9-yn-1-yl ethyl ester

Inchi: InChI=1S/C18H30O4/c1-3-5-6-7-8-9-10-11-12-13-16-22-18(20)15-14-17(19)21-4-2/h3-4,
InchiKey: NSMIPLPWRAYALI-UHFFFAOYSA-N
Formula: C18H30O4
SMILES: CCC#CCCCCCCCCOC(=O)CCC(=O)OCC
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-164.36	kJ/mol	Joback Method
hf	-632.15	kJ/mol	Joback Method
hfus	51.07	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.017		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
tb	772.82	K	Joback Method
tc	961.42	K	Joback Method
tf	543.04	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.97	J/mol×K	772.82	Joback Method
cpg	818.65	J/mol×K	804.25	Joback Method
cpg	834.39	J/mol×K	835.69	Joback Method
cpg	849.21	J/mol×K	867.12	Joback Method
cpg	863.12	J/mol×K	898.55	Joback Method
cpg	876.12	J/mol×K	929.99	Joback Method
cpg	888.23	J/mol×K	961.42	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=U391004&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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