Succinic acid, but-3-yn-2-yl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C20H30O4/c1-4-6-7-8-9-10-11-12-13-14-17-23-19(21)15-16-20(22)24-18(3)5-2

InchiKey: LPIYQZYMNORFCL-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: C#CC(C)OC(=O)CCC(=O)OCCCCCCCCCC#CCC

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	73.11	kJ/mol	Joback Method
hf	-386.81	kJ/mol	Joback Method
hfus	55.70	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.019		Crippen Method
mcvol	290.340	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2333.00		NIST Webbook
tb	808.26	K	Joback Method
tc	1004.89	K	Joback Method
tf	597.55	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.93	J/mol×K	808.26	Joback Method
cpg	881.50	J/mol×K	841.03	Joback Method
cpg	897.06	J/mol×K	873.80	Joback Method
cpg	911.63	J/mol×K	906.57	Joback Method
cpg	925.23	J/mol×K	939.34	Joback Method
cpg	937.88	J/mol×K	972.12	Joback Method
cpg	949.61	J/mol×K	1004.89	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=U390994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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