Succinic acid, tridec-2-yn-1-yl trans-hex-3-en-1-yl ester

Inchi: InChI=1S/C23H38O4/c1-3-5-7-9-10-11-12-13-14-15-17-21-27-23(25)19-18-22(24)26-20-

InchiKey: HZWRTEIZCVZLLG-SOFGYWHQSA-N

Formula: C23H38O4

SMILES: CCC=CCCOC(=O)CCC(=O)OCC#CCCCCCCCCCC

Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-42.04	kJ/mol	Joback Method
hf	-618.13	kJ/mol	Joback Method
hfus	64.22	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.743		Crippen Method
mcvol	336.910	ml/mol	McGowan Method
pc	1025.97	kPa	Joback Method
rinpol	2694.00		NIST Webbook
rinpol	2694.00		NIST Webbook
tb	891.38	K	Joback Method
tc	1092.62	K	Joback Method
tf	594.31	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.54	J/mol×K	891.38	Joback Method
cpg	1093.40	J/mol×K	924.92	Joback Method
cpg	1110.11	J/mol×K	958.46	Joback Method
cpg	1125.70	J/mol×K	992.00	Joback Method
cpg	1140.21	J/mol×K	1025.54	Joback Method
cpg	1153.68	J/mol×K	1059.08	Joback Method
cpg	1166.14	J/mol×K	1092.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391126&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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