Succinic acid, tridec-2-yn-1-yl pent-4-en-1-yl ester

Inchi: InChI=1S/C22H36O4/c1-3-5-7-8-9-10-11-12-13-14-16-20-26-22(24)18-17-21(23)25-19-1
InchiKey: GKTYFDHIJCXROQ-UHFFFAOYSA-N
Formula: C22H36O4
SMILES: C=CCCCOC(=O)CCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-42.84	kJ/mol	Joback Method
hf	-589.28	kJ/mol	Joback Method
hfus	60.15	kJ/mol	Joback Method
hvap	84.36	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.353		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	861.02	K	Joback Method
tc	1057.00	K	Joback Method
tf	586.36	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.93	J/mol×K	861.02	Joback Method
cpg	1030.42	J/mol×K	893.68	Joback Method
cpg	1046.79	J/mol×K	926.35	Joback Method
cpg	1062.07	J/mol×K	959.01	Joback Method
cpg	1076.28	J/mol×K	991.67	Joback Method
cpg	1089.45	J/mol×K	1024.34	Joback Method
cpg	1101.59	J/mol×K	1057.00	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=U391077&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