Succinic acid, tridec-2-yn-1-yl cis-pent-2-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: CRPRDQVMZUPBGV-UUASQNMZSA-N

Formula: C22H36O4

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

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-50.46	kJ/mol	Joback Method
hf	-597.49	kJ/mol	Joback Method
hfus	61.63	kJ/mol	Joback Method
hvap	84.99	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.353		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1092.10	kPa	Joback Method
rinpol	2628.00		NIST Webbook
tb	868.50	K	Joback Method
tc	1066.59	K	Joback Method
tf	583.04	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.31	J/mol×K	868.50	Joback Method
cpg	1031.82	J/mol×K	901.52	Joback Method
cpg	1048.23	J/mol×K	934.53	Joback Method
cpg	1063.58	J/mol×K	967.55	Joback Method
cpg	1077.90	J/mol×K	1000.56	Joback Method
cpg	1091.22	J/mol×K	1033.58	Joback Method
cpg	1103.58	J/mol×K	1066.59	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=U391272&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