Succinic acid, tridec-2-yn-1-yl cyclopentyl ester

Inchi: InChI=1S/C22H36O4/c1-2-3-4-5-6-7-8-9-10-11-14-19-25-21(23)17-18-22(24)26-20-15-12

InchiKey: YGQYYBWVBREAHW-UHFFFAOYSA-N

Formula: C22H36O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OC1CCCC1

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-94.13	kJ/mol	Joback Method
hf	-654.23	kJ/mol	Joback Method
hfus	55.37	kJ/mol	Joback Method
hvap	85.29	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.330		Crippen Method
mcvol	316.260	ml/mol	McGowan Method
pc	1190.70	kPa	Joback Method
rinpol	2737.00		NIST Webbook
rinpol	2737.00		NIST Webbook
tb	879.62	K	Joback Method
tc	1084.53	K	Joback Method
tf	599.02	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.16	J/mol×K	879.62	Joback Method
cpg	1051.35	J/mol×K	913.77	Joback Method
cpg	1068.24	J/mol×K	947.92	Joback Method
cpg	1083.85	J/mol×K	982.08	Joback Method
cpg	1098.22	J/mol×K	1016.23	Joback Method
cpg	1111.38	J/mol×K	1050.38	Joback Method
cpg	1123.36	J/mol×K	1084.53	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=U391386&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