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

Inchi: InChI=1S/C22H36O4/c1-4-5-6-7-8-9-10-11-12-13-14-18-25-21(23)15-16-22(24)26-19-17

InchiKey: PQFBRZDDXAANQT-UHFFFAOYSA-N

Formula: C22H36O4

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

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-51.39	kJ/mol	Joback Method
hf	-599.07	kJ/mol	Joback Method
hfus	58.84	kJ/mol	Joback Method
hvap	84.44	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.353		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1088.50	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	860.90	K	Joback Method
tc	1057.63	K	Joback Method
tf	572.40	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.54	J/mol×K	860.90	Joback Method
cpg	1030.11	J/mol×K	893.69	Joback Method
cpg	1046.55	J/mol×K	926.48	Joback Method
cpg	1061.89	J/mol×K	959.27	Joback Method
cpg	1076.16	J/mol×K	992.06	Joback Method
cpg	1089.39	J/mol×K	1024.85	Joback Method
cpg	1101.60	J/mol×K	1057.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391147&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