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

Inchi: InChI=1S/C26H44O4/c1-3-5-7-9-11-12-13-14-16-18-20-24-30-26(28)22-21-25(27)29-23-

InchiKey: CSRYTSWYKJKQNC-BMRADRMJSA-N

Formula: C26H44O4

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

Mol. weight [g/mol]: 420.63

Physical Properties

Property code	Value	Unit	Source
gf	-16.78	kJ/mol	Joback Method
hf	-680.05	kJ/mol	Joback Method
hfus	71.99	kJ/mol	Joback Method
hvap	93.89	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	6.914		Crippen Method
mcvol	379.180	ml/mol	McGowan Method
pc	859.99	kPa	Joback Method
rinpol	2994.00		NIST Webbook
tb	960.02	K	Joback Method
tc	1176.26	K	Joback Method
tf	628.12	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.91	J/mol×K	960.02	Joback Method
cpg	1282.02	J/mol×K	996.06	Joback Method
cpg	1299.75	J/mol×K	1032.10	Joback Method
cpg	1316.14	J/mol×K	1068.14	Joback Method
cpg	1331.25	J/mol×K	1104.18	Joback Method
cpg	1345.14	J/mol×K	1140.22	Joback Method
cpg	1357.87	J/mol×K	1176.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391105&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

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