Succinic acid, tridec-2-yn-1-yl 3-phenylpropyl ester

Inchi: InChI=1S/C26H38O4/c1-2-3-4-5-6-7-8-9-10-11-15-22-29-25(27)20-21-26(28)30-23-16-19

InchiKey: MNQIHPXYKQJRFC-UHFFFAOYSA-N

Formula: C26H38O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	15.41	kJ/mol	Joback Method
hf	-560.74	kJ/mol	Joback Method
hfus	65.83	kJ/mol	Joback Method
hvap	96.21	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.020		Crippen Method
mcvol	359.720	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	3172.00		NIST Webbook
rinpol	3172.00		NIST Webbook
tb	982.54	K	Joback Method
tc	1203.28	K	Joback Method
tf	659.62	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.11	J/mol×K	982.54	Joback Method
cpg	1204.53	J/mol×K	1019.33	Joback Method
cpg	1219.50	J/mol×K	1056.12	Joback Method
cpg	1233.07	J/mol×K	1092.91	Joback Method
cpg	1245.30	J/mol×K	1129.70	Joback Method
cpg	1256.23	J/mol×K	1166.49	Joback Method
cpg	1265.93	J/mol×K	1203.28	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=U389738&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