Sebacic acid, di(2,7-dimethylocta-7-en-5-yn-4-yl) ester

Inchi: InChI=1S/C30H46O4/c1-23(2)17-19-27(21-25(5)6)33-29(31)15-13-11-9-10-12-14-16-30(

InchiKey: RWCRNVDNRCOPEL-UHFFFAOYSA-N

Formula: C30H46O4

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OC(C#CC(=C)C)CC(C)C

Mol. weight [g/mol]: 470.68

Physical Properties

Property code	Value	Unit	Source
gf	288.30	kJ/mol	Joback Method
hf	-397.37	kJ/mol	Joback Method
hfus	66.00	kJ/mol	Joback Method
hvap	102.26	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	7.182		Crippen Method
mcvol	422.640	ml/mol	McGowan Method
pc	789.04	kPa	Joback Method
rinpol	2381.00		NIST Webbook
tb	1047.74	K	Joback Method
tc	1283.38	K	Joback Method
tf	692.94	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1428.77	J/mol×K	1047.74	Joback Method
cpg	1446.86	J/mol×K	1087.01	Joback Method
cpg	1463.31	J/mol×K	1126.29	Joback Method
cpg	1478.18	J/mol×K	1165.56	Joback Method
cpg	1491.56	J/mol×K	1204.83	Joback Method
cpg	1503.52	J/mol×K	1244.10	Joback Method
cpg	1514.14	J/mol×K	1283.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355819&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