Sebacic acid, di(2,6-dimethylnon-1-en-3-yn-5-yl) ester

Inchi: InChI=1S/C32H50O4/c1-9-17-27(7)29(23-21-25(3)4)35-31(33)19-15-13-11-12-14-16-20-

InchiKey: JBOWKLYFDXLJPV-UHFFFAOYSA-N

Formula: C32H50O4

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

Mol. weight [g/mol]: 498.74

Physical Properties

Property code	Value	Unit	Source
gf	305.14	kJ/mol	Joback Method
hf	-438.65	kJ/mol	Joback Method
hfus	71.18	kJ/mol	Joback Method
hvap	106.71	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	7.962		Crippen Method
mcvol	450.820	ml/mol	McGowan Method
pc	710.35	kPa	Joback Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook
tb	1093.50	K	Joback Method
tc	1344.31	K	Joback Method
tf	715.48	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1556.66	J/mol×K	1093.50	Joback Method
cpg	1575.34	J/mol×K	1135.30	Joback Method
cpg	1592.16	J/mol×K	1177.10	Joback Method
cpg	1607.23	J/mol×K	1218.90	Joback Method
cpg	1620.65	J/mol×K	1260.70	Joback Method
cpg	1632.52	J/mol×K	1302.51	Joback Method
cpg	1642.94	J/mol×K	1344.31	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=U355813&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