Sebacic acid, 2,6-dimethylnon-1-en-3-yn-5-yl nonyl ester

Inchi: InChI=1S/C30H52O4/c1-6-8-9-10-13-16-19-25-33-29(31)21-17-14-11-12-15-18-22-30(32

InchiKey: ZWICGRZLBUZRES-UHFFFAOYSA-N

Formula: C30H52O4

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

Mol. weight [g/mol]: 476.73

Physical Properties

Property code	Value	Unit	Source
gf	11.09	kJ/mol	Joback Method
hf	-774.75	kJ/mol	Joback Method
hfus	72.52	kJ/mol	Joback Method
hvap	101.47	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	8.329		Crippen Method
mcvol	435.540	ml/mol	McGowan Method
pc	698.76	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	1043.06	K	Joback Method
tc	1287.99	K	Joback Method
tf	632.56	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1517.19	J/mol×K	1043.06	Joback Method
cpg	1537.76	J/mol×K	1083.88	Joback Method
cpg	1556.37	J/mol×K	1124.70	Joback Method
cpg	1573.11	J/mol×K	1165.53	Joback Method
cpg	1588.06	J/mol×K	1206.35	Joback Method
cpg	1601.32	J/mol×K	1247.17	Joback Method
cpg	1612.96	J/mol×K	1287.99	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=U355811&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