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

Inchi: InChI=1S/C29H50O4/c1-6-8-9-10-15-18-24-32-28(30)20-16-13-11-12-14-17-21-29(31)33

InchiKey: PCLLCYBBVNKYAX-UHFFFAOYSA-N

Formula: C29H50O4

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

Mol. weight [g/mol]: 462.70

Physical Properties

Property code	Value	Unit	Source
gf	2.67	kJ/mol	Joback Method
hf	-754.11	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	99.25	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	7.938		Crippen Method
mcvol	421.450	ml/mol	McGowan Method
pc	735.62	kPa	Joback Method
rinpol	3014.00		NIST Webbook
tb	1020.18	K	Joback Method
tc	1255.40	K	Joback Method
tf	621.29	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1452.74	J/mol×K	1020.18	Joback Method
cpg	1472.83	J/mol×K	1059.38	Joback Method
cpg	1491.10	J/mol×K	1098.59	Joback Method
cpg	1507.65	J/mol×K	1137.79	Joback Method
cpg	1522.54	J/mol×K	1176.99	Joback Method
cpg	1535.84	J/mol×K	1216.20	Joback Method
cpg	1547.63	J/mol×K	1255.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355810&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