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

Inchi: InChI=1S/C27H46O4/c1-6-8-9-16-22-30-26(28)18-14-12-10-11-13-15-19-27(29)31-25(21

InchiKey: FEZRBCQYTMBKCJ-UHFFFAOYSA-N

Formula: C27H46O4

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

Mol. weight [g/mol]: 434.65

Physical Properties

Property code	Value	Unit	Source
gf	-14.17	kJ/mol	Joback Method
hf	-712.83	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	94.79	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.158		Crippen Method
mcvol	393.270	ml/mol	McGowan Method
pc	818.66	kPa	Joback Method
rinpol	2811.00		NIST Webbook
tb	974.42	K	Joback Method
tc	1194.01	K	Joback Method
tf	598.75	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1324.88	J/mol×K	974.42	Joback Method
cpg	1344.12	J/mol×K	1011.02	Joback Method
cpg	1361.81	J/mol×K	1047.62	Joback Method
cpg	1377.99	J/mol×K	1084.22	Joback Method
cpg	1392.72	J/mol×K	1120.82	Joback Method
cpg	1406.06	J/mol×K	1157.41	Joback Method
cpg	1418.06	J/mol×K	1194.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355808&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