Sebacic acid, 2,7-dimethylocta-7-en-5-yn-4-yl pentyl ester

Inchi: InChI=1S/C25H42O4/c1-6-7-14-19-28-24(26)15-12-10-8-9-11-13-16-25(27)29-23(20-22(

InchiKey: IPUORNVPIGOMDU-UHFFFAOYSA-N

Formula: C25H42O4

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

Mol. weight [g/mol]: 406.60

Physical Properties

Property code	Value	Unit	Source
gf	-31.01	kJ/mol	Joback Method
hf	-671.55	kJ/mol	Joback Method
hfus	59.57	kJ/mol	Joback Method
hvap	90.34	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.378		Crippen Method
mcvol	365.090	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	928.66	K	Joback Method
tc	1137.11	K	Joback Method
tf	576.21	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.70	J/mol×K	928.66	Joback Method
cpg	1217.25	J/mol×K	963.40	Joback Method
cpg	1234.43	J/mol×K	998.14	Joback Method
cpg	1250.29	J/mol×K	1032.88	Joback Method
cpg	1264.86	J/mol×K	1067.63	Joback Method
cpg	1278.17	J/mol×K	1102.37	Joback Method
cpg	1290.28	J/mol×K	1137.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355816&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