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

Inchi: InChI=1S/C24H40O4/c1-6-14-21(5)22(18-17-20(3)4)28-24(26)16-13-11-9-8-10-12-15-23

InchiKey: CZHFIUYROWYSGZ-UHFFFAOYSA-N

Formula: C24H40O4

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

Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-39.43	kJ/mol	Joback Method
hf	-650.91	kJ/mol	Joback Method
hfus	56.98	kJ/mol	Joback Method
hvap	88.12	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.988		Crippen Method
mcvol	351.000	ml/mol	McGowan Method
pc	972.30	kPa	Joback Method
rinpol	2533.00		NIST Webbook
tb	905.78	K	Joback Method
tc	1110.14	K	Joback Method
tf	564.94	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.37	J/mol×K	905.78	Joback Method
cpg	1154.62	J/mol×K	939.84	Joback Method
cpg	1171.58	J/mol×K	973.90	Joback Method
cpg	1187.28	J/mol×K	1007.96	Joback Method
cpg	1201.76	J/mol×K	1042.02	Joback Method
cpg	1215.06	J/mol×K	1076.08	Joback Method
cpg	1227.20	J/mol×K	1110.14	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=U355804&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