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

Inchi: InChI=1S/C28H48O4/c1-6-8-9-14-17-23-31-27(29)19-15-12-10-11-13-16-20-28(30)32-26

InchiKey: ATFDHOVOYGVREB-UHFFFAOYSA-N

Formula: C28H48O4

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

Mol. weight [g/mol]: 448.68

Physical Properties

Property code	Value	Unit	Source
gf	-5.75	kJ/mol	Joback Method
hf	-733.47	kJ/mol	Joback Method
hfus	67.34	kJ/mol	Joback Method
hvap	97.02	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.548		Crippen Method
mcvol	407.360	ml/mol	McGowan Method
pc	775.48	kPa	Joback Method
rinpol	2912.00		NIST Webbook
rinpol	2912.00		NIST Webbook
tb	997.30	K	Joback Method
tc	1224.10	K	Joback Method
tf	610.02	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1388.63	J/mol×K	997.30	Joback Method
cpg	1408.27	J/mol×K	1035.10	Joback Method
cpg	1426.24	J/mol×K	1072.90	Joback Method
cpg	1442.60	J/mol×K	1110.70	Joback Method
cpg	1457.41	J/mol×K	1148.50	Joback Method
cpg	1470.74	J/mol×K	1186.30	Joback Method
cpg	1482.64	J/mol×K	1224.10	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=U355809&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