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

Inchi: InChI=1S/C26H44O4/c1-6-8-15-21-29-25(27)17-13-11-9-10-12-14-18-26(28)30-24(20-19

InchiKey: XQWLMLFZVAXHFW-UHFFFAOYSA-N

Formula: C26H44O4

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

Mol. weight [g/mol]: 420.63

Physical Properties

Property code	Value	Unit	Source
gf	-22.59	kJ/mol	Joback Method
hf	-692.19	kJ/mol	Joback Method
hfus	62.16	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	6.768		Crippen Method
mcvol	379.180	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	2714.00		NIST Webbook
tb	951.54	K	Joback Method
tc	1165.04	K	Joback Method
tf	587.48	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1261.56	J/mol×K	951.54	Joback Method
cpg	1280.43	J/mol×K	987.12	Joback Method
cpg	1297.86	J/mol×K	1022.71	Joback Method
cpg	1313.87	J/mol×K	1058.29	Joback Method
cpg	1328.52	J/mol×K	1093.87	Joback Method
cpg	1341.86	J/mol×K	1129.46	Joback Method
cpg	1353.92	J/mol×K	1165.04	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355807&Units=SI

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