Sebacic acid, 2-methyloct-5-yn-4-yl octyl ester

Inchi: InChI=1S/C27H48O4/c1-5-7-9-10-15-18-22-30-26(28)20-16-13-11-12-14-17-21-27(29)31
InchiKey: QFVAMJVNRXCVEA-UHFFFAOYSA-N
Formula: C27H48O4
SMILES: CCC#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-93.46	kJ/mol	Joback Method
hf	-828.47	kJ/mol	Joback Method
hfus	67.34	kJ/mol	Joback Method
hvap	95.38	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.382		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	797.08	kPa	Joback Method
rinpol	2901.00		NIST Webbook
tb	977.86	K	Joback Method
tc	1199.72	K	Joback Method
tf	614.47	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.24	J/mol×K	977.86	Joback Method
cpg	1375.00	J/mol×K	1014.84	Joback Method
cpg	1393.10	J/mol×K	1051.81	Joback Method
cpg	1409.57	J/mol×K	1088.79	Joback Method
cpg	1424.46	J/mol×K	1125.76	Joback Method
cpg	1437.83	J/mol×K	1162.74	Joback Method
cpg	1449.72	J/mol×K	1199.72	Joback Method

Sources

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=U355872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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