Glutaric acid, but-3-yn-2-yl octadecyl ester

Inchi: InChI=1S/C27H48O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-30-26(28)22-2
InchiKey: ZKXCFNDLGTVASS-UHFFFAOYSA-N
Formula: C27H48O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-70.75	kJ/mol	Joback Method
hf	-803.59	kJ/mol	Joback Method
hfus	70.71	kJ/mol	Joback Method
hvap	93.48	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.526		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	788.16	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	959.42	K	Joback Method
tc	1178.87	K	Joback Method
tf	570.34	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.70	J/mol×K	959.42	Joback Method
cpg	1368.05	J/mol×K	996.00	Joback Method
cpg	1386.83	J/mol×K	1032.57	Joback Method
cpg	1404.10	J/mol×K	1069.15	Joback Method
cpg	1419.91	J/mol×K	1105.72	Joback Method
cpg	1434.34	J/mol×K	1142.30	Joback Method
cpg	1447.43	J/mol×K	1178.87	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=U391643&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