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

Inchi: InChI=1S/C23H40O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-20-26-22(24)18-17-19-23(25)2
InchiKey: HUDNVSSLASIIQU-UHFFFAOYSA-N
Formula: C23H40O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-104.43	kJ/mol	Joback Method
hf	-721.03	kJ/mol	Joback Method
hfus	60.35	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.966		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	2622.00		NIST Webbook
tb	867.90	K	Joback Method
tc	1063.14	K	Joback Method
tf	525.26	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.15	J/mol×K	867.90	Joback Method
cpg	1114.58	J/mol×K	900.44	Joback Method
cpg	1131.84	J/mol×K	932.98	Joback Method
cpg	1147.95	J/mol×K	965.52	Joback Method
cpg	1162.96	J/mol×K	998.06	Joback Method
cpg	1176.88	J/mol×K	1030.60	Joback Method
cpg	1189.75	J/mol×K	1063.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359885&Units=SI
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

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