Glutaric acid, but-3-yn-2-yl undec-2-enyl ester

Inchi: InChI=1S/C20H32O4/c1-4-6-7-8-9-10-11-12-13-17-23-19(21)15-14-16-20(22)24-18(3)5-2
InchiKey: DNLRHLDDOFFZMN-OUKQBFOZSA-N
Formula: C20H32O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC=CCCCCCCCC
Mol. weight [g/mol]: 336.47

Physical Properties

Property code	Value	Unit	Source
gf	-49.47	kJ/mol	Joback Method
hf	-541.89	kJ/mol	Joback Method
hfus	52.78	kJ/mol	Joback Method
hvap	77.85	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.572		Crippen Method
mcvol	294.640	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	803.42	K	Joback Method
tc	993.44	K	Joback Method
tf	486.37	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.99	J/mol×K	803.42	Joback Method
cpg	905.78	J/mol×K	835.09	Joback Method
cpg	921.61	J/mol×K	866.76	Joback Method
cpg	936.52	J/mol×K	898.43	Joback Method
cpg	950.53	J/mol×K	930.10	Joback Method
cpg	963.68	J/mol×K	961.77	Joback Method
cpg	976.01	J/mol×K	993.44	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=U394013&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