Glutaric acid, but-3-yn-2-yl hex-4-yn-3-yl ester

Inchi: InChI=1S/C15H20O4/c1-5-9-13(7-3)19-15(17)11-8-10-14(16)18-12(4)6-2/h2,12-13H,7-8,
InchiKey: RMQGRIRMTUSBHJ-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	28.57	kJ/mol	Joback Method
hf	-288.89	kJ/mol	Joback Method
hfus	39.23	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.067		Crippen Method
mcvol	219.890	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	693.42	K	Joback Method
tc	899.12	K	Joback Method
tf	526.20	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.46	J/mol×K	693.42	Joback Method
cpg	600.53	J/mol×K	727.70	Joback Method
cpg	614.74	J/mol×K	761.99	Joback Method
cpg	628.10	J/mol×K	796.27	Joback Method
cpg	640.63	J/mol×K	830.55	Joback Method
cpg	652.32	J/mol×K	864.83	Joback Method
cpg	663.19	J/mol×K	899.12	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=U393972&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