Glutaric acid, hex-4-yn-3-yl but-3-en-1-yl ester

Inchi: InChI=1S/C15H22O4/c1-4-7-12-18-14(16)10-8-11-15(17)19-13(6-3)9-5-2/h4,13H,1,6-8,1
InchiKey: WLWJFPBIPBUKGT-UHFFFAOYSA-N
Formula: C15H22O4
SMILES: C=CCCOC(=O)CCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-104.22	kJ/mol	Joback Method
hf	-450.08	kJ/mol	Joback Method
hfus	38.50	kJ/mol	Joback Method
hvap	68.39	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.621		Crippen Method
mcvol	224.190	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	1810.00		NIST Webbook
tb	700.42	K	Joback Method
tc	895.74	K	Joback Method
tf	492.47	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.30	J/mol×K	700.42	Joback Method
cpg	624.54	J/mol×K	732.97	Joback Method
cpg	638.96	J/mol×K	765.53	Joback Method
cpg	652.56	J/mol×K	798.08	Joback Method
cpg	665.35	J/mol×K	830.63	Joback Method
cpg	677.34	J/mol×K	863.18	Joback Method
cpg	688.54	J/mol×K	895.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394035&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