Glutaric acid, hex-2-en-1-yl but-3-yn-2-yl ester

Inchi: InChI=1S/C15H22O4/c1-4-6-7-8-12-18-14(16)10-9-11-15(17)19-13(3)5-2/h2,7-8,13H,4,6
InchiKey: PTIJHXAOGWVMAU-BQYQJAHWSA-N
Formula: C15H22O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC=CCCC
Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-91.57	kJ/mol	Joback Method
hf	-438.69	kJ/mol	Joback Method
hfus	39.83	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.621		Crippen Method
mcvol	224.190	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1748.00		NIST Webbook
rinpol	1748.00		NIST Webbook
tb	689.02	K	Joback Method
tc	880.20	K	Joback Method
tf	430.02	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.86	J/mol×K	689.02	Joback Method
cpg	621.73	J/mol×K	720.88	Joback Method
cpg	635.81	J/mol×K	752.75	Joback Method
cpg	649.12	J/mol×K	784.61	Joback Method
cpg	661.69	J/mol×K	816.47	Joback Method
cpg	673.52	J/mol×K	848.33	Joback Method
cpg	684.65	J/mol×K	880.20	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=U405326&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