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

Inchi: InChI=1S/C14H20O4/c1-4-6-7-11-17-13(15)9-8-10-14(16)18-12(3)5-2/h2,6-7,12H,4,8-11
InchiKey: LMZNUADNUCTIBI-VOTSOKGWSA-N
Formula: C14H20O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC=CCC
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-99.99	kJ/mol	Joback Method
hf	-418.05	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.231		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	666.14	K	Joback Method
tc	859.01	K	Joback Method
tf	418.75	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.93	J/mol×K	666.14	Joback Method
cpg	568.31	J/mol×K	698.28	Joback Method
cpg	581.93	J/mol×K	730.43	Joback Method
cpg	594.82	J/mol×K	762.57	Joback Method
cpg	606.99	J/mol×K	794.72	Joback Method
cpg	618.45	J/mol×K	826.86	Joback Method
cpg	629.23	J/mol×K	859.01	Joback Method

Sources

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=U405254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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