Glutaric acid, but-3-yn-2-yl pentyl ester

Inchi: InChI=1S/C14H22O4/c1-4-6-7-11-17-13(15)9-8-10-14(16)18-12(3)5-2/h2,12H,4,6-11H2,1
InchiKey: QNPXAXSIIFAROH-UHFFFAOYSA-N
Formula: C14H22O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-180.21	kJ/mol	Joback Method
hf	-535.27	kJ/mol	Joback Method
hfus	37.04	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.455		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	1718.00		NIST Webbook
tb	661.98	K	Joback Method
tc	848.46	K	Joback Method
tf	423.83	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.92	J/mol×K	661.98	Joback Method
cpg	590.82	J/mol×K	693.06	Joback Method
cpg	604.97	J/mol×K	724.14	Joback Method
cpg	618.39	J/mol×K	755.22	Joback Method
cpg	631.09	J/mol×K	786.30	Joback Method
cpg	643.08	J/mol×K	817.38	Joback Method
cpg	654.36	J/mol×K	848.46	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=U359875&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