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

Inchi: InChI=1S/C14H22O4/c1-5-12(4)18-14(16)8-6-7-13(15)17-10-9-11(2)3/h1,11-12H,6-10H2
InchiKey: UALDRQFXDCPENW-UHFFFAOYSA-N
Formula: C14H22O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCC(C)C
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-182.65	kJ/mol	Joback Method
hf	-540.55	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.311		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
tb	661.54	K	Joback Method
tc	851.00	K	Joback Method
tf	408.83	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.39	J/mol×K	661.54	Joback Method
cpg	591.56	J/mol×K	693.12	Joback Method
cpg	605.95	J/mol×K	724.69	Joback Method
cpg	619.58	J/mol×K	756.27	Joback Method
cpg	632.46	J/mol×K	787.85	Joback Method
cpg	644.59	J/mol×K	819.43	Joback Method
cpg	655.98	J/mol×K	851.00	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=U392544&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