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

Inchi: InChI=1S/C13H20O4/c1-5-11(4)17-13(15)8-6-7-12(14)16-9-10(2)3/h1,10-11H,6-9H2,2-4
InchiKey: PRLVZJOLCQXAPI-UHFFFAOYSA-N
Formula: C13H20O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-191.07	kJ/mol	Joback Method
hf	-519.91	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	61.93	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.921		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1580.00		NIST Webbook
tb	638.66	K	Joback Method
tc	829.97	K	Joback Method
tf	397.56	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.25	J/mol×K	638.66	Joback Method
cpg	538.88	J/mol×K	670.54	Joback Method
cpg	552.78	J/mol×K	702.43	Joback Method
cpg	565.96	J/mol×K	734.31	Joback Method
cpg	578.41	J/mol×K	766.20	Joback Method
cpg	590.16	J/mol×K	798.08	Joback Method
cpg	601.20	J/mol×K	829.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359873&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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