Glutaric acid, di(but-3-yn-2-yl) ester

Inchi: InChI=1S/C13H16O4/c1-5-10(3)16-12(14)8-7-9-13(15)17-11(4)6-2/h1-2,10-11H,7-9H2,3-
InchiKey: MEAKCWZVIFPMNT-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC(C)C#C
Mol. weight [g/mol]: 236.26

Physical Properties

Property code	Value	Unit	Source
gf	32.00	kJ/mol	Joback Method
hf	-228.01	kJ/mol	Joback Method
hfus	33.90	kJ/mol	Joback Method
hvap	61.78	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.286		Crippen Method
mcvol	191.710	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
tb	628.78	K	Joback Method
tc	831.29	K	Joback Method
tf	444.53	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.47	J/mol×K	628.78	Joback Method
cpg	493.96	J/mol×K	662.53	Joback Method
cpg	506.72	J/mol×K	696.28	Joback Method
cpg	518.77	J/mol×K	730.04	Joback Method
cpg	530.11	J/mol×K	763.79	Joback Method
cpg	540.76	J/mol×K	797.54	Joback Method
cpg	550.73	J/mol×K	831.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359887&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

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