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

Inchi: InChI=1S/C11H16O4/c1-4-9(3)15-11(13)8-6-7-10(12)14-5-2/h1,9H,5-8H2,2-3H3
InchiKey: OYNRAJCEBASJIZ-UHFFFAOYSA-N
Formula: C11H16O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCC
Mol. weight [g/mol]: 212.24

Physical Properties

Property code	Value	Unit	Source
gf	-205.47	kJ/mol	Joback Method
hf	-473.35	kJ/mol	Joback Method
hfus	29.27	kJ/mol	Joback Method
hvap	57.86	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.285		Crippen Method
mcvol	172.130	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
tb	593.34	K	Joback Method
tc	785.57	K	Joback Method
tf	390.02	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.99	J/mol×K	593.34	Joback Method
cpg	437.01	J/mol×K	625.38	Joback Method
cpg	449.43	J/mol×K	657.42	Joback Method
cpg	461.23	J/mol×K	689.45	Joback Method
cpg	472.44	J/mol×K	721.49	Joback Method
cpg	483.04	J/mol×K	753.53	Joback Method
cpg	493.05	J/mol×K	785.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359871&Units=SI

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