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

Inchi: InChI=1S/C12H18O4/c1-4-9-15-11(13)7-6-8-12(14)16-10(3)5-2/h2,10H,4,6-9H2,1,3H3
InchiKey: DAWILSNFMOZBRU-UHFFFAOYSA-N
Formula: C12H18O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCC
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	-197.05	kJ/mol	Joback Method
hf	-493.99	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	60.09	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.675		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1521.00		NIST Webbook
tb	616.22	K	Joback Method
tc	806.23	K	Joback Method
tf	401.29	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.11	J/mol×K	616.22	Joback Method
cpg	486.84	J/mol×K	647.89	Joback Method
cpg	499.91	J/mol×K	679.56	Joback Method
cpg	512.34	J/mol×K	711.23	Joback Method
cpg	524.11	J/mol×K	742.90	Joback Method
cpg	535.25	J/mol×K	774.56	Joback Method
cpg	545.74	J/mol×K	806.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359872&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