Glutaric acid, but-3-yn-2-yl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C17H28O4/c1-7-14(3)21-16(19)10-8-9-15(18)20-12-13(2)11-17(4,5)6/h1,13-14

InchiKey: OTXFIJQIHMEIMO-UHFFFAOYSA-N

Formula: C17H28O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-154.55	kJ/mol	Joback Method
hf	-611.22	kJ/mol	Joback Method
hfus	33.88	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.337		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	726.95	K	Joback Method
tc	920.18	K	Joback Method
tf	445.06	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.71	J/mol×K	726.95	Joback Method
cpg	759.49	J/mol×K	759.15	Joback Method
cpg	775.30	J/mol×K	791.36	Joback Method
cpg	790.16	J/mol×K	823.56	Joback Method
cpg	804.12	J/mol×K	855.77	Joback Method
cpg	817.20	J/mol×K	887.97	Joback Method
cpg	829.42	J/mol×K	920.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391525&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