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

Inchi: InChI=1S/C17H18O5/c1-4-12(2)21-16(19)6-5-7-17(20)22-15-10-8-14(9-11-15)13(3)18/h1

InchiKey: ONYJGXNTHYXRIG-UHFFFAOYSA-N

Formula: C17H18O5

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 302.32

Physical Properties

Property code	Value	Unit	Source
gf	-181.09	kJ/mol	Joback Method
hf	-484.71	kJ/mol	Joback Method
hfus	40.06	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	2.530		Crippen Method
mcvol	234.480	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook
tb	816.15	K	Joback Method
tc	1034.74	K	Joback Method
tf	546.51	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.88	J/mol×K	816.15	Joback Method
cpg	679.85	J/mol×K	852.58	Joback Method
cpg	691.76	J/mol×K	889.01	Joback Method
cpg	702.63	J/mol×K	925.44	Joback Method
cpg	712.48	J/mol×K	961.88	Joback Method
cpg	721.34	J/mol×K	998.31	Joback Method
cpg	729.21	J/mol×K	1034.74	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=U392030&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