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

Inchi: InChI=1S/C16H18O4/c1-4-13(3)19-15(17)9-6-10-16(18)20-14-8-5-7-12(2)11-14/h1,5,7-8

InchiKey: FKLJBYJCKPWDID-UHFFFAOYSA-N

Formula: C16H18O4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-60.59	kJ/mol	Joback Method
hf	-351.49	kJ/mol	Joback Method
hfus	35.87	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	2.636		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	739.40	K	Joback Method
tc	954.59	K	Joback Method
tf	485.31	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.35	J/mol×K	739.40	Joback Method
cpg	612.76	J/mol×K	775.26	Joback Method
cpg	626.17	J/mol×K	811.13	Joback Method
cpg	638.60	J/mol×K	846.99	Joback Method
cpg	650.08	J/mol×K	882.86	Joback Method
cpg	660.61	J/mol×K	918.72	Joback Method
cpg	670.23	J/mol×K	954.59	Joback Method

Sources

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=U391949&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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