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

Inchi: InChI=1S/C21H20O4/c1-3-16(2)24-20(22)10-7-11-21(23)25-19-14-12-18(13-15-19)17-8-
InchiKey: ZDYXZHVMCNVKPU-UHFFFAOYSA-N
Formula: C21H20O4
SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	93.92	kJ/mol	Joback Method
hf	-218.16	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	85.34	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	3.994		Crippen Method
mcvol	265.510	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2662.00		NIST Webbook
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tb	880.48	K	Joback Method
tc	1114.80	K	Joback Method
tf	568.08	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.60	J/mol×K	880.48	Joback Method
cpg	796.32	J/mol×K	919.53	Joback Method
cpg	808.73	J/mol×K	958.59	Joback Method
cpg	819.91	J/mol×K	997.64	Joback Method
cpg	829.89	J/mol×K	1036.69	Joback Method
cpg	838.74	J/mol×K	1075.74	Joback Method
cpg	846.51	J/mol×K	1114.80	Joback Method

Sources

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=U390119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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