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

Inchi: InChI=1S/C22H22O4/c1-3-17(2)25-20(23)15-10-16-21(24)26-22(18-11-6-4-7-12-18)19-1
InchiKey: LXNAPQKUUORICJ-UHFFFAOYSA-N
Formula: C22H22O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	109.53	kJ/mol	Joback Method
hf	-232.61	kJ/mol	Joback Method
hfus	42.32	kJ/mol	Joback Method
hvap	86.51	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.054		Crippen Method
mcvol	279.600	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2509.00		NIST Webbook
tb	897.94	K	Joback Method
tc	1132.20	K	Joback Method
tf	551.83	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.82	J/mol×K	897.94	Joback Method
cpg	855.86	J/mol×K	936.98	Joback Method
cpg	868.56	J/mol×K	976.03	Joback Method
cpg	879.97	J/mol×K	1015.07	Joback Method
cpg	890.19	J/mol×K	1054.12	Joback Method
cpg	899.26	J/mol×K	1093.16	Joback Method
cpg	907.27	J/mol×K	1132.20	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=U393339&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