Glutaric acid, hex-4-yn-3-yl diphenylmethyl ester

Inchi: InChI=1S/C24H26O4/c1-3-12-21(4-2)27-22(25)17-11-18-23(26)28-24(19-13-7-5-8-14-19)20-15-9-6-10-16-20/h5-10,13-16,21,24H,4,11,17-18H2,1-2H3

InchiKey: KSSSUPGJXUGSLK-UHFFFAOYSA-N

Formula: C24H26O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OC(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 378.46

Physical Properties

Property code	Value	Unit	Source
gf	106.10	kJ/mol	Joback Method
hf	-293.49	kJ/mol	Joback Method
hfus	47.65	kJ/mol	Joback Method
hvap	93.26	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	4.835		Crippen Method
mcvol	307.780	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2761.00		NIST Webbook
rinpol	2761.00		NIST Webbook
tb	962.58	K	Joback Method
tc	1200.23	K	Joback Method
tf	633.50	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.26	J/mol×K	962.58	Joback Method
cpg	976.18	J/mol×K	1002.19	Joback Method
cpg	988.63	J/mol×K	1041.80	Joback Method
cpg	999.66	J/mol×K	1081.41	Joback Method
cpg	1009.35	J/mol×K	1121.01	Joback Method
cpg	1017.75	J/mol×K	1160.62	Joback Method
cpg	1024.94	J/mol×K	1200.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393343&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