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

Inchi: InChI=1S/C17H20O4/c1-3-14(2)21-17(19)11-7-10-16(18)20-13-12-15-8-5-4-6-9-15/h1,4-
InchiKey: QSCVUFNECKYCKC-UHFFFAOYSA-N
Formula: C17H20O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-42.54	kJ/mol	Joback Method
hf	-360.66	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	73.49	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.507		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook
tb	757.30	K	Joback Method
tc	969.03	K	Joback Method
tf	484.06	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.79	J/mol×K	757.30	Joback Method
cpg	668.63	J/mol×K	792.59	Joback Method
cpg	682.43	J/mol×K	827.88	Joback Method
cpg	695.22	J/mol×K	863.17	Joback Method
cpg	707.02	J/mol×K	898.46	Joback Method
cpg	717.87	J/mol×K	933.75	Joback Method
cpg	727.78	J/mol×K	969.03	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=U391786&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

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