Glutaric acid, but-3-yn-2-yl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C17H20O6/c1-5-12(2)22-15(18)10-7-11-16(19)23-17-13(20-3)8-6-9-14(17)21-4

InchiKey: FSMRGUGMWRELBU-UHFFFAOYSA-N

Formula: C17H20O6

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 320.34

Physical Properties

Property code	Value	Unit	Source
gf	-271.80	kJ/mol	Joback Method
hf	-648.04	kJ/mol	Joback Method
hfus	40.45	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.344		Crippen Method
mcvol	244.650	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	2259.00		NIST Webbook
rinpol	2259.00		NIST Webbook
tb	812.10	K	Joback Method
tc	1023.06	K	Joback Method
tf	553.56	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.19	J/mol×K	812.10	Joback Method
cpg	719.95	J/mol×K	847.26	Joback Method
cpg	732.61	J/mol×K	882.42	Joback Method
cpg	744.13	J/mol×K	917.58	Joback Method
cpg	754.52	J/mol×K	952.74	Joback Method
cpg	763.75	J/mol×K	987.90	Joback Method
cpg	771.82	J/mol×K	1023.06	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=U391998&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