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

Inchi: InChI=1S/C17H20O4/c1-5-13(3)20-16(18)10-7-11-17(19)21-15-9-6-8-12(2)14(15)4/h1,6,8

InchiKey: ALKXMKZHFVMLJA-UHFFFAOYSA-N

Formula: C17H20O4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-61.80	kJ/mol	Joback Method
hf	-383.60	kJ/mol	Joback Method
hfus	38.07	kJ/mol	Joback Method
hvap	74.82	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	2.944		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	767.26	K	Joback Method
tc	980.56	K	Joback Method
tf	509.10	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.85	J/mol×K	767.26	Joback Method
cpg	666.48	J/mol×K	802.81	Joback Method
cpg	680.09	J/mol×K	838.36	Joback Method
cpg	692.71	J/mol×K	873.91	Joback Method
cpg	704.35	J/mol×K	909.46	Joback Method
cpg	715.02	J/mol×K	945.01	Joback Method
cpg	724.74	J/mol×K	980.56	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=U392214&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