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

Inchi: InChI=1S/C18H22O4/c1-5-14(4)21-17(19)11-8-12-18(20)22-16-10-7-6-9-15(16)13(2)3/h1

InchiKey: XZTGKVSFFUYXNO-UHFFFAOYSA-N

Formula: C18H22O4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 302.36

Physical Properties

Property code	Value	Unit	Source
gf	-46.19	kJ/mol	Joback Method
hf	-398.05	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	75.99	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.451		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	784.72	K	Joback Method
tc	998.14	K	Joback Method
tf	492.85	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.93	J/mol×K	784.72	Joback Method
cpg	724.15	J/mol×K	820.29	Joback Method
cpg	738.28	J/mol×K	855.86	Joback Method
cpg	751.33	J/mol×K	891.43	Joback Method
cpg	763.35	J/mol×K	927.00	Joback Method
cpg	774.34	J/mol×K	962.57	Joback Method
cpg	784.34	J/mol×K	998.14	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=U391912&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