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

Inchi: InChI=1S/C18H22O5/c1-5-14(4)22-17(19)11-8-12-18(20)23-16-10-7-6-9-15(16)21-13(2)3

InchiKey: LIHDIPIUYUMPDC-UHFFFAOYSA-N

Formula: C18H22O5

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 318.36

Physical Properties

Property code	Value	Unit	Source
gf	-151.19	kJ/mol	Joback Method
hf	-530.27	kJ/mol	Joback Method
hfus	38.72	kJ/mol	Joback Method
hvap	78.40	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.114		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	807.14	K	Joback Method
tc	1019.40	K	Joback Method
tf	515.08	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.64	J/mol×K	807.14	Joback Method
cpg	751.38	J/mol×K	842.52	Joback Method
cpg	764.98	J/mol×K	877.89	Joback Method
cpg	777.45	J/mol×K	913.27	Joback Method
cpg	788.81	J/mol×K	948.65	Joback Method
cpg	799.06	J/mol×K	984.02	Joback Method
cpg	808.22	J/mol×K	1019.40	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=U391866&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