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

Inchi: InChI=1S/C16H18O5/c1-4-12(2)20-15(17)10-7-11-16(18)21-14-9-6-5-8-13(14)19-3/h1,5-

InchiKey: JYDRXWPSYKDYAL-UHFFFAOYSA-N

Formula: C16H18O5

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

Mol. weight [g/mol]: 290.31

Physical Properties

Property code	Value	Unit	Source
gf	-165.59	kJ/mol	Joback Method
hf	-483.71	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	74.34	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.336		Crippen Method
mcvol	224.690	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2086.00		NIST Webbook
rinpol	2086.00		NIST Webbook
tb	761.82	K	Joback Method
tc	975.19	K	Joback Method
tf	507.54	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.02	J/mol×K	761.82	Joback Method
cpg	639.05	J/mol×K	797.38	Joback Method
cpg	652.05	J/mol×K	832.94	Joback Method
cpg	664.04	J/mol×K	868.51	Joback Method
cpg	675.02	J/mol×K	904.07	Joback Method
cpg	684.98	J/mol×K	939.63	Joback Method
cpg	693.95	J/mol×K	975.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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