Glutaric acid, but-3-yn-2-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C16H17FO5/c1-4-11(2)21-15(18)6-5-7-16(19)22-13-9-8-12(17)10-14(13)20-3/h

InchiKey: FPGOGMNITMZOJZ-UHFFFAOYSA-N

Formula: C16H17FO5

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 308.30

Physical Properties

Property code	Value	Unit	Source
gf	-370.03	kJ/mol	Joback Method
hf	-691.29	kJ/mol	Joback Method
hfus	39.75	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.475		Crippen Method
mcvol	226.460	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	766.07	K	Joback Method
tc	972.92	K	Joback Method
tf	520.65	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.64	J/mol×K	766.07	Joback Method
cpg	645.00	J/mol×K	800.54	Joback Method
cpg	657.41	J/mol×K	835.02	Joback Method
cpg	668.87	J/mol×K	869.49	Joback Method
cpg	679.38	J/mol×K	903.97	Joback Method
cpg	688.94	J/mol×K	938.44	Joback Method
cpg	697.55	J/mol×K	972.92	Joback Method

Sources

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=U393439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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