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

Inchi: InChI=1S/C15H15FO4/c1-3-11(2)19-14(17)8-5-9-15(18)20-13-7-4-6-12(16)10-13/h1,4,6-

InchiKey: LJUCPGNZNKNEIU-UHFFFAOYSA-N

Formula: C15H15FO4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 278.28

Physical Properties

Property code	Value	Unit	Source
gf	-263.82	kJ/mol	Joback Method
hf	-526.96	kJ/mol	Joback Method
hfus	36.36	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.466		Crippen Method
mcvol	206.500	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	715.79	K	Joback Method
tc	925.59	K	Joback Method
tf	474.63	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.91	J/mol×K	715.79	Joback Method
cpg	566.30	J/mol×K	750.76	Joback Method
cpg	578.79	J/mol×K	785.72	Joback Method
cpg	590.40	J/mol×K	820.69	Joback Method
cpg	601.13	J/mol×K	855.66	Joback Method
cpg	611.01	J/mol×K	890.62	Joback Method
cpg	620.06	J/mol×K	925.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392086&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