Glutaric acid, hex-4-yn-3-yl 3-fluorophenyl ester

Inchi: InChI=1S/C17H19FO4/c1-3-7-14(4-2)21-16(19)10-6-11-17(20)22-15-9-5-8-13(18)12-15/h

InchiKey: OEFBFBJWIXTRSM-UHFFFAOYSA-N

Formula: C17H19FO4

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

Mol. weight [g/mol]: 306.33

Physical Properties

Property code	Value	Unit	Source
gf	-267.25	kJ/mol	Joback Method
hf	-587.84	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.246		Crippen Method
mcvol	234.680	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	780.43	K	Joback Method
tc	993.22	K	Joback Method
tf	556.30	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.54	J/mol×K	780.43	Joback Method
cpg	677.97	J/mol×K	815.89	Joback Method
cpg	691.34	J/mol×K	851.36	Joback Method
cpg	703.69	J/mol×K	886.82	Joback Method
cpg	715.02	J/mol×K	922.29	Joback Method
cpg	725.34	J/mol×K	957.75	Joback Method
cpg	734.66	J/mol×K	993.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392091&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

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