Glutaric acid, but-3-yn-2-yl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C16H26O5/c1-5-14(3)21-16(18)8-6-7-15(17)20-12-10-13(2)9-11-19-4/h1,13-14

InchiKey: AZRHCVDZTDIOEG-UHFFFAOYSA-N

Formula: C16H26O5

SMILES: C#CC(C)OC(=O)CCCC(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 298.37

Physical Properties

Property code	Value	Unit	Source
gf	-270.81	kJ/mol	Joback Method
hf	-714.05	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	71.01	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.328		Crippen Method
mcvol	248.450	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	729.72	K	Joback Method
tc	916.65	K	Joback Method
tf	453.60	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.51	J/mol×K	729.72	Joback Method
cpg	729.29	J/mol×K	760.88	Joback Method
cpg	744.20	J/mol×K	792.03	Joback Method
cpg	758.24	J/mol×K	823.19	Joback Method
cpg	771.43	J/mol×K	854.34	Joback Method
cpg	783.75	J/mol×K	885.50	Joback Method
cpg	795.22	J/mol×K	916.65	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=U393517&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