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

Inchi: InChI=1S/C17H28O4/c1-5-8-9-11-15(7-3)21-17(19)13-10-12-16(18)20-14(4)6-2/h2,14-15
InchiKey: JCRLECCFOTZASL-UHFFFAOYSA-N
Formula: C17H28O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OC(CC)CCCCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-157.39	kJ/mol	Joback Method
hf	-602.47	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.624		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook
tb	730.18	K	Joback Method
tc	916.54	K	Joback Method
tf	442.64	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.63	J/mol×K	730.18	Joback Method
cpg	757.06	J/mol×K	761.24	Joback Method
cpg	772.60	J/mol×K	792.30	Joback Method
cpg	787.27	J/mol×K	823.36	Joback Method
cpg	801.08	J/mol×K	854.42	Joback Method
cpg	814.04	J/mol×K	885.48	Joback Method
cpg	826.18	J/mol×K	916.54	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=U391555&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