Glutaric acid, hexa-1,5-dien-3-yl hex-4-yn-3-yl ester

Inchi: InChI=1S/C17H24O4/c1-5-10-14(7-3)20-16(18)12-9-13-17(19)21-15(8-4)11-6-2/h5,7,14-
InchiKey: KSOWJGUBICFRHQ-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-1.98	kJ/mol	Joback Method
hf	-371.21	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	71.78	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.176		Crippen Method
mcvol	248.070	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	742.42	K	Joback Method
tc	940.27	K	Joback Method
tf	498.25	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.21	J/mol×K	742.42	Joback Method
cpg	710.94	J/mol×K	775.40	Joback Method
cpg	725.74	J/mol×K	808.37	Joback Method
cpg	739.64	J/mol×K	841.35	Joback Method
cpg	752.64	J/mol×K	874.32	Joback Method
cpg	764.78	J/mol×K	907.30	Joback Method
cpg	776.05	J/mol×K	940.27	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=U405278&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