Glutaric acid, hex-4-yn-3-yl cis-hex-3-enyl ester

Inchi: InChI=1S/C17H26O4/c1-4-7-8-9-14-20-16(18)12-10-13-17(19)21-15(6-3)11-5-2/h7-8,15H

InchiKey: SWOXRQBHHSGLHO-FPLPWBNLSA-N

Formula: C17H26O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCC=CCC

Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	-95.00	kJ/mol	Joback Method
hf	-499.57	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	73.47	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.401		Crippen Method
mcvol	252.370	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	753.66	K	Joback Method
tc	949.59	K	Joback Method
tf	511.69	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.79	J/mol×K	753.66	Joback Method
cpg	736.83	J/mol×K	786.31	Joback Method
cpg	751.96	J/mol×K	818.97	Joback Method
cpg	766.21	J/mol×K	851.62	Joback Method
cpg	779.58	J/mol×K	884.28	Joback Method
cpg	792.11	J/mol×K	916.93	Joback Method
cpg	803.79	J/mol×K	949.59	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=U394027&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