Glutaric acid, 3,4-dimethylcyclohexyl but-3-yn-2-yl ester

Inchi: InChI=1S/C17H26O4/c1-5-14(4)20-16(18)7-6-8-17(19)21-15-10-9-12(2)13(3)11-15/h1,12

InchiKey: OMPFQFIOJOKGJR-UHFFFAOYSA-N

Formula: C17H26O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OC1CCC(C)C(C)C1

Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	-145.92	kJ/mol	Joback Method
hf	-583.55	kJ/mol	Joback Method
hfus	38.79	kJ/mol	Joback Method
hvap	71.03	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.089		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	740.83	K	Joback Method
tc	947.19	K	Joback Method
tf	456.54	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.43	J/mol×K	740.83	Joback Method
cpg	759.37	J/mol×K	775.22	Joback Method
cpg	777.07	J/mol×K	809.62	Joback Method
cpg	793.51	J/mol×K	844.01	Joback Method
cpg	808.71	J/mol×K	878.40	Joback Method
cpg	822.69	J/mol×K	912.80	Joback Method
cpg	835.44	J/mol×K	947.19	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=U405430&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