Glutaric acid, 2-(cyclohexyl)ethyl but-3-yn-2-yl ester

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

InchiKey: VYVWKMLYXZCBAS-UHFFFAOYSA-N

Formula: C17H26O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	-130.50	kJ/mol	Joback Method
hf	-542.87	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	71.65	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.235		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook
tb	750.17	K	Joback Method
tc	956.79	K	Joback Method
tf	465.02	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.01	J/mol×K	750.17	Joback Method
cpg	753.03	J/mol×K	784.61	Joback Method
cpg	769.86	J/mol×K	819.04	Joback Method
cpg	785.50	J/mol×K	853.48	Joback Method
cpg	799.98	J/mol×K	887.92	Joback Method
cpg	813.32	J/mol×K	922.36	Joback Method
cpg	825.55	J/mol×K	956.79	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=U405414&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