Glutaric acid, 1-cyclopentylethyl but-3-yn-2-yl ester

Inchi: InChI=1S/C16H24O4/c1-4-12(2)19-15(17)10-7-11-16(18)20-13(3)14-8-5-6-9-14/h1,12-14

InchiKey: COZUVVUHCZMCLF-UHFFFAOYSA-N

Formula: C16H24O4

SMILES: C#CC(C)OC(=O)CCCC(=O)OC(C)C1CCCC1

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-129.26	kJ/mol	Joback Method
hf	-521.35	kJ/mol	Joback Method
hfus	32.63	kJ/mol	Joback Method
hvap	68.86	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.843		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	722.58	K	Joback Method
tc	929.38	K	Joback Method
tf	442.27	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.71	J/mol×K	722.58	Joback Method
cpg	693.23	J/mol×K	757.05	Joback Method
cpg	709.63	J/mol×K	791.51	Joback Method
cpg	724.94	J/mol×K	825.98	Joback Method
cpg	739.18	J/mol×K	860.45	Joback Method
cpg	752.39	J/mol×K	894.92	Joback Method
cpg	764.58	J/mol×K	929.38	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=U405457&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