Glutaric acid, 1-cyclopentylethyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C18H28O4/c1-4-9-16(5-2)22-18(20)13-8-12-17(19)21-14(3)15-10-6-7-11-15/h1

InchiKey: QJLKWHRFYSOUML-UHFFFAOYSA-N

Formula: C18H28O4

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

Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-132.69	kJ/mol	Joback Method
hf	-582.23	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	75.61	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.624		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
tb	787.22	K	Joback Method
tc	997.43	K	Joback Method
tf	523.94	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.72	J/mol×K	787.22	Joback Method
cpg	812.88	J/mol×K	822.25	Joback Method
cpg	829.79	J/mol×K	857.29	Joback Method
cpg	845.47	J/mol×K	892.32	Joback Method
cpg	859.95	J/mol×K	927.36	Joback Method
cpg	873.26	J/mol×K	962.39	Joback Method
cpg	885.41	J/mol×K	997.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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