Glutaric acid, cyclohexylmethyl hex-4-yn-3-yl ester

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

InchiKey: AHYKYOUCDZNQNB-UHFFFAOYSA-N

Formula: C18H28O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-142.35	kJ/mol	Joback Method
hf	-583.11	kJ/mol	Joback Method
hfus	39.38	kJ/mol	Joback Method
hvap	76.17	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.625		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	791.93	K	Joback Method
tc	1004.07	K	Joback Method
tf	535.42	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.01	J/mol×K	791.93	Joback Method
cpg	816.41	J/mol×K	827.29	Joback Method
cpg	833.47	J/mol×K	862.64	Joback Method
cpg	849.23	J/mol×K	898.00	Joback Method
cpg	863.69	J/mol×K	933.36	Joback Method
cpg	876.88	J/mol×K	968.72	Joback Method
cpg	888.81	J/mol×K	1004.07	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=U393978&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