Glutaric acid, 2,7-dimethyloct-5-yn-7-en-4-yl propyl ester

Inchi: InChI=1S/C18H28O4/c1-6-12-21-17(19)8-7-9-18(20)22-16(13-15(4)5)11-10-14(2)3/h15-1

InchiKey: MNAOAXLWKTYAQF-UHFFFAOYSA-N

Formula: C18H28O4

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

Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-89.95	kJ/mol	Joback Method
hf	-527.07	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	74.76	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.647		Crippen Method
mcvol	266.460	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	1990.00		NIST Webbook
tb	768.50	K	Joback Method
tc	965.12	K	Joback Method
tf	497.32	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.81	J/mol×K	768.50	Joback Method
cpg	793.51	J/mol×K	801.27	Joback Method
cpg	809.23	J/mol×K	834.04	Joback Method
cpg	823.98	J/mol×K	866.81	Joback Method
cpg	837.76	J/mol×K	899.58	Joback Method
cpg	850.60	J/mol×K	932.35	Joback Method
cpg	862.51	J/mol×K	965.12	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=U359835&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