Glutaric acid, hexa-1,5-dien-3-yl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C24H38O4/c1-4-7-8-9-10-11-12-13-14-15-16-21-27-23(25)19-17-20-24(26)28-

InchiKey: BIUSWQXTURENPE-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OCC#CCCCCCCCCCC

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	59.40	kJ/mol	Joback Method
hf	-510.41	kJ/mol	Joback Method
hfus	60.53	kJ/mol	Joback Method
hvap	87.75	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	5.908		Crippen Method
mcvol	346.700	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook
tb	903.02	K	Joback Method
tc	1106.42	K	Joback Method
tf	592.14	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.53	J/mol×K	903.02	Joback Method
cpg	1125.23	J/mol×K	936.92	Joback Method
cpg	1141.71	J/mol×K	970.82	Joback Method
cpg	1157.01	J/mol×K	1004.72	Joback Method
cpg	1171.16	J/mol×K	1038.62	Joback Method
cpg	1184.22	J/mol×K	1072.52	Joback Method
cpg	1196.20	J/mol×K	1106.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405290&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