Glutaric acid, cyclopentyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C23H38O4/c1-2-3-4-5-6-7-8-9-10-11-14-20-26-22(24)18-15-19-23(25)27-21-16
InchiKey: KDCXAHMSJQDQCM-UHFFFAOYSA-N
Formula: C23H38O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OC1CCCC1
Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-85.71	kJ/mol	Joback Method
hf	-674.87	kJ/mol	Joback Method
hfus	57.96	kJ/mol	Joback Method
hvap	87.51	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.720		Crippen Method
mcvol	330.350	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinpol	2768.00		NIST Webbook
rinpol	2768.00		NIST Webbook
tb	902.50	K	Joback Method
tc	1109.31	K	Joback Method
tf	610.29	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.76	J/mol×K	902.50	Joback Method
cpg	1113.09	J/mol×K	936.97	Joback Method
cpg	1130.07	J/mol×K	971.44	Joback Method
cpg	1145.72	J/mol×K	1005.91	Joback Method
cpg	1160.09	J/mol×K	1040.37	Joback Method
cpg	1173.21	J/mol×K	1074.84	Joback Method
cpg	1185.12	J/mol×K	1109.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405403&Units=SI

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