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

Inchi: InChI=1S/C25H42O4/c1-3-4-5-6-7-8-9-10-11-12-15-21-28-24(26)19-16-20-25(27)29-22(2

InchiKey: ASQRASOMOGHTKF-UHFFFAOYSA-N

Formula: C25H42O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OC(C)C1CCCC1

Mol. weight [g/mol]: 406.60

Physical Properties

Property code	Value	Unit	Source
gf	-71.31	kJ/mol	Joback Method
hf	-721.43	kJ/mol	Joback Method
hfus	59.61	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.356		Crippen Method
mcvol	358.530	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	2883.00		NIST Webbook
rinpol	2883.00		NIST Webbook
tb	947.82	K	Joback Method
tc	1161.39	K	Joback Method
tf	617.83	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.00	J/mol×K	947.82	Joback Method
cpg	1238.67	J/mol×K	983.41	Joback Method
cpg	1255.83	J/mol×K	1019.01	Joback Method
cpg	1271.54	J/mol×K	1054.60	Joback Method
cpg	1285.83	J/mol×K	1090.20	Joback Method
cpg	1298.76	J/mol×K	1125.79	Joback Method
cpg	1310.38	J/mol×K	1161.39	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=U405472&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