Glutaric acid, 3,4-dimethylcyclohexyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C26H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-20-29-25(27)16-15-17-26(28)30-24
InchiKey: BQJQDGOHURVYSI-UHFFFAOYSA-N
Formula: C26H44O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OC1CCC(C)C(C)C1
Mol. weight [g/mol]: 420.63

Physical Properties

Property code	Value	Unit	Source
gf	-87.97	kJ/mol	Joback Method
hf	-783.63	kJ/mol	Joback Method
hfus	65.77	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.602		Crippen Method
mcvol	372.620	ml/mol	McGowan Method
pc	905.61	kPa	Joback Method
rinpol	3022.00		NIST Webbook
rinpol	3022.00		NIST Webbook
tb	966.07	K	Joback Method
tc	1183.04	K	Joback Method
tf	632.10	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1295.22	J/mol×K	966.07	Joback Method
cpg	1314.12	J/mol×K	1002.23	Joback Method
cpg	1331.18	J/mol×K	1038.39	Joback Method
cpg	1346.45	J/mol×K	1074.55	Joback Method
cpg	1359.94	J/mol×K	1110.71	Joback Method
cpg	1371.69	J/mol×K	1146.88	Joback Method
cpg	1381.72	J/mol×K	1183.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405435&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

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