Glutaric acid, tridec-2-yn-1-yl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C26H38O6/c1-4-5-6-7-8-9-10-11-12-13-14-21-31-24(27)19-16-20-25(28)32-26

InchiKey: VRPKZCCCNSXSGP-UHFFFAOYSA-N

Formula: C26H38O6

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 446.58

Physical Properties

Property code	Value	Unit	Source
gf	-213.85	kJ/mol	Joback Method
hf	-848.12	kJ/mol	Joback Method
hfus	67.43	kJ/mol	Joback Method
hvap	102.35	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	5.857		Crippen Method
mcvol	371.460	ml/mol	McGowan Method
pc	979.62	kPa	Joback Method
rinpol	3278.00		NIST Webbook
rinpol	3278.00		NIST Webbook
tb	1037.34	K	Joback Method
tc	1270.63	K	Joback Method
tf	729.12	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.35	J/mol×K	1037.34	Joback Method
cpg	1256.35	J/mol×K	1076.22	Joback Method
cpg	1268.35	J/mol×K	1115.10	Joback Method
cpg	1278.34	J/mol×K	1153.98	Joback Method
cpg	1286.34	J/mol×K	1192.87	Joback Method
cpg	1292.35	J/mol×K	1231.75	Joback Method
cpg	1296.37	J/mol×K	1270.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392012&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