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

Inchi: InChI=1S/C27H40O5/c1-4-5-6-7-8-9-10-11-12-13-16-22-30-26(28)20-17-21-27(29)32-25
InchiKey: OHACZWSVEKKENW-UHFFFAOYSA-N
Formula: C27H40O5
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 444.60

Physical Properties

Property code	Value	Unit	Source
gf	-93.24	kJ/mol	Joback Method
hf	-730.35	kJ/mol	Joback Method
hfus	65.70	kJ/mol	Joback Method
hvap	101.12	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.627		Crippen Method
mcvol	379.680	ml/mol	McGowan Method
pc	946.16	kPa	Joback Method
rinpol	3173.00		NIST Webbook
tb	1032.38	K	Joback Method
tc	1264.21	K	Joback Method
tf	690.64	K	Joback Method
vc	1.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.96	J/mol×K	1032.38	Joback Method
cpg	1293.30	J/mol×K	1071.02	Joback Method
cpg	1306.84	J/mol×K	1109.66	Joback Method
cpg	1318.60	J/mol×K	1148.30	Joback Method
cpg	1328.62	J/mol×K	1186.94	Joback Method
cpg	1336.94	J/mol×K	1225.57	Joback Method
cpg	1343.59	J/mol×K	1264.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391878&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