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

Inchi: InChI=1S/C25H36O4/c1-3-4-5-6-7-8-9-10-11-12-15-21-28-24(26)19-16-20-25(27)29-23-1

InchiKey: DITDUYXAYBHXNM-UHFFFAOYSA-N

Formula: C25H36O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccccc1C

Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-2.64	kJ/mol	Joback Method
hf	-551.57	kJ/mol	Joback Method
hfus	62.85	kJ/mol	Joback Method
hvap	94.65	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	6.148		Crippen Method
mcvol	345.630	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	2996.00		NIST Webbook
rinpol	2996.00		NIST Webbook
tb	964.64	K	Joback Method
tc	1182.62	K	Joback Method
tf	660.87	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.74	J/mol×K	964.64	Joback Method
cpg	1141.87	J/mol×K	1000.97	Joback Method
cpg	1156.58	J/mol×K	1037.30	Joback Method
cpg	1169.92	J/mol×K	1073.63	Joback Method
cpg	1181.93	J/mol×K	1109.96	Joback Method
cpg	1192.66	J/mol×K	1146.29	Joback Method
cpg	1202.13	J/mol×K	1182.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391819&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