Glutaric acid, tridec-2-yn-1-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C26H38O4/c1-4-5-6-7-8-9-10-11-12-13-14-21-29-25(27)19-16-20-26(28)30-24

InchiKey: SYTGAAYVSCHMHQ-UHFFFAOYSA-N

Formula: C26H38O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	-3.85	kJ/mol	Joback Method
hf	-583.68	kJ/mol	Joback Method
hfus	65.06	kJ/mol	Joback Method
hvap	97.53	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.457		Crippen Method
mcvol	359.720	ml/mol	McGowan Method
pc	1000.81	kPa	Joback Method
rinpol	3134.00		NIST Webbook
tb	992.50	K	Joback Method
tc	1215.37	K	Joback Method
tf	684.66	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.62	J/mol×K	992.50	Joback Method
cpg	1202.76	J/mol×K	1029.64	Joback Method
cpg	1217.39	J/mol×K	1066.79	Joback Method
cpg	1230.55	J/mol×K	1103.93	Joback Method
cpg	1242.26	J/mol×K	1141.08	Joback Method
cpg	1252.57	J/mol×K	1178.22	Joback Method
cpg	1261.52	J/mol×K	1215.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392229&Units=SI

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