Glutaric acid, tridec-2-yn-1-yl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C25H35ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-19-29-24(27)15-14-16-25(28)30-23

InchiKey: ZHSMQLVHNAFJMA-UHFFFAOYSA-N

Formula: C25H35ClO4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 435.00

Physical Properties

Property code	Value	Unit	Source
gf	-24.20	kJ/mol	Joback Method
hf	-578.78	kJ/mol	Joback Method
hfus	66.66	kJ/mol	Joback Method
hvap	99.69	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	6.802		Crippen Method
mcvol	357.870	ml/mol	McGowan Method
pc	1039.24	kPa	Joback Method
rinpol	3207.00		NIST Webbook
rinpol	3207.00		NIST Webbook
tb	1007.05	K	Joback Method
tc	1233.35	K	Joback Method
tf	703.31	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.60	J/mol×K	1007.05	Joback Method
cpg	1164.34	J/mol×K	1044.77	Joback Method
cpg	1177.59	J/mol×K	1082.48	Joback Method
cpg	1189.41	J/mol×K	1120.20	Joback Method
cpg	1199.84	J/mol×K	1157.92	Joback Method
cpg	1208.90	J/mol×K	1195.63	Joback Method
cpg	1216.65	J/mol×K	1233.35	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=U392081&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