Glutaric acid, tridec-2-yn-1-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C25H35ClO5/c1-3-4-5-6-7-8-9-10-11-12-13-19-30-24(27)15-14-16-25(28)31-22

InchiKey: HMNQTZLTUGTAEN-UHFFFAOYSA-N

Formula: C25H35ClO5

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 451.00

Physical Properties

Property code	Value	Unit	Source
gf	-129.20	kJ/mol	Joback Method
hf	-711.00	kJ/mol	Joback Method
hfus	67.85	kJ/mol	Joback Method
hvap	102.10	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.502		Crippen Method
mcvol	363.740	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	3280.00		NIST Webbook
rinpol	3280.00		NIST Webbook
tb	1029.47	K	Joback Method
tc	1260.36	K	Joback Method
tf	725.54	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.83	J/mol×K	1029.47	Joback Method
cpg	1190.51	J/mol×K	1067.95	Joback Method
cpg	1202.50	J/mol×K	1106.43	Joback Method
cpg	1212.80	J/mol×K	1144.92	Joback Method
cpg	1221.45	J/mol×K	1183.40	Joback Method
cpg	1228.46	J/mol×K	1221.88	Joback Method
cpg	1233.86	J/mol×K	1260.36	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=U393916&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