Glutaric acid, but-3-yn-2-yl 2-chlorophenyl ester

Inchi: InChI=1S/C15H15ClO4/c1-3-11(2)19-14(17)9-6-10-15(18)20-13-8-5-4-7-12(13)16/h1,4-5

InchiKey: RAWGXOPRUIQTHU-UHFFFAOYSA-N

Formula: C15H15ClO4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 294.73

Physical Properties

Property code	Value	Unit	Source
gf	-80.94	kJ/mol	Joback Method
hf	-346.59	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	2.981		Crippen Method
mcvol	216.970	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	753.95	K	Joback Method
tc	975.25	K	Joback Method
tf	503.96	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.69	J/mol×K	753.95	Joback Method
cpg	582.57	J/mol×K	790.83	Joback Method
cpg	594.47	J/mol×K	827.72	Joback Method
cpg	605.42	J/mol×K	864.60	Joback Method
cpg	615.44	J/mol×K	901.48	Joback Method
cpg	624.55	J/mol×K	938.37	Joback Method
cpg	632.77	J/mol×K	975.25	Joback Method

Sources

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=U391883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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