Glutaric acid, but-3-yn-2-yl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C16H17ClO4/c1-4-12(3)20-15(18)6-5-7-16(19)21-14-9-8-13(17)10-11(14)2/h1,

InchiKey: BTWVRKVYELJRKW-UHFFFAOYSA-N

Formula: C16H17ClO4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 308.76

Physical Properties

Property code	Value	Unit	Source
gf	-82.15	kJ/mol	Joback Method
hf	-378.70	kJ/mol	Joback Method
hfus	39.68	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.289		Crippen Method
mcvol	231.060	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	781.81	K	Joback Method
tc	1000.88	K	Joback Method
tf	527.75	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.18	J/mol×K	781.81	Joback Method
cpg	635.33	J/mol×K	818.32	Joback Method
cpg	647.48	J/mol×K	854.83	Joback Method
cpg	658.67	J/mol×K	891.34	Joback Method
cpg	668.89	J/mol×K	927.86	Joback Method
cpg	678.18	J/mol×K	964.37	Joback Method
cpg	686.53	J/mol×K	1000.88	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=U392064&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