Glutaric acid, but-3-yn-2-yl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C15H14ClFO4/c1-3-10(2)20-13(18)8-5-9-14(19)21-15-11(16)6-4-7-12(15)17/h1

InchiKey: GCRIWMOZZCAZNK-UHFFFAOYSA-N

Formula: C15H14ClFO4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 312.72

Physical Properties

Property code	Value	Unit	Source
gf	-285.38	kJ/mol	Joback Method
hf	-554.17	kJ/mol	Joback Method
hfus	40.17	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.120		Crippen Method
mcvol	218.740	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2001.00		NIST Webbook
tb	758.20	K	Joback Method
tc	972.08	K	Joback Method
tf	517.07	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.15	J/mol×K	758.20	Joback Method
cpg	588.36	J/mol×K	793.85	Joback Method
cpg	599.67	J/mol×K	829.49	Joback Method
cpg	610.10	J/mol×K	865.14	Joback Method
cpg	619.67	J/mol×K	900.78	Joback Method
cpg	628.38	J/mol×K	936.43	Joback Method
cpg	636.24	J/mol×K	972.08	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=U391578&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