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

Inchi: InChI=1S/C9H11ClO3/c1-3-7(2)13-9(12)6-4-5-8(10)11/h1,7H,4-6H2,2H3
InchiKey: SDRKDDWJROHQEO-UHFFFAOYSA-N
Formula: C9H11ClO3
SMILES: C#CC(C)OC(=O)CCCC(=O)Cl
Mol. weight [g/mol]: 202.63

Physical Properties

Property code	Value	Unit	Source
gf	-129.24	kJ/mol	Joback Method
hf	-315.59	kJ/mol	Joback Method
hfus	27.10	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.487		Crippen Method
mcvol	150.320	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1311.00		NIST Webbook
tb	562.59	K	Joback Method
tc	766.19	K	Joback Method
tf	375.17	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.58	J/mol×K	562.59	Joback Method
cpg	343.38	J/mol×K	596.52	Joback Method
cpg	353.60	J/mol×K	630.46	Joback Method
cpg	363.27	J/mol×K	664.39	Joback Method
cpg	372.39	J/mol×K	698.33	Joback Method
cpg	380.98	J/mol×K	732.26	Joback Method
cpg	389.04	J/mol×K	766.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359888&Units=SI
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

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