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

Inchi: InChI=1S/C11H14Cl2O4/c1-3-8(2)17-11(15)6-4-5-10(14)16-7-9(12)13/h1,8-9H,4-7H2,2H

InchiKey: RONXAWQBQWRUJQ-UHFFFAOYSA-N

Formula: C11H14Cl2O4

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

Mol. weight [g/mol]: 281.13

Physical Properties

Property code	Value	Unit	Source
gf	-231.77	kJ/mol	Joback Method
hf	-510.11	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.068		Crippen Method
mcvol	196.610	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	667.76	K	Joback Method
tc	871.39	K	Joback Method
tf	434.86	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.00	J/mol×K	667.76	Joback Method
cpg	487.74	J/mol×K	701.70	Joback Method
cpg	498.78	J/mol×K	735.64	Joback Method
cpg	509.14	J/mol×K	769.57	Joback Method
cpg	518.81	J/mol×K	803.51	Joback Method
cpg	527.82	J/mol×K	837.45	Joback Method
cpg	536.15	J/mol×K	871.39	Joback Method

Sources

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=U393995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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