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

Inchi: InChI=1S/C15H14Cl2O4/c1-3-10(2)20-13(18)8-5-9-14(19)21-12-7-4-6-11(16)15(12)17/h1

InchiKey: ITCNIDZVMCQKAB-UHFFFAOYSA-N

Formula: C15H14Cl2O4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 329.18

Physical Properties

Property code	Value	Unit	Source
gf	-102.50	kJ/mol	Joback Method
hf	-373.80	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.634		Crippen Method
mcvol	229.210	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	796.36	K	Joback Method
tc	1021.30	K	Joback Method
tf	546.40	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.18	J/mol×K	796.36	Joback Method
cpg	602.81	J/mol×K	833.85	Joback Method
cpg	613.49	J/mol×K	871.34	Joback Method
cpg	623.21	J/mol×K	908.83	Joback Method
cpg	632.01	J/mol×K	946.32	Joback Method
cpg	639.90	J/mol×K	983.81	Joback Method
cpg	646.89	J/mol×K	1021.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394004&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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