Glutaric acid, 2,4,6-trichlorophenyl but-3-yn-2-yl ester

Inchi: InChI=1S/C15H13Cl3O4/c1-3-9(2)21-13(19)5-4-6-14(20)22-15-11(17)7-10(16)8-12(15)18

InchiKey: CAYARHVETACCTP-UHFFFAOYSA-N

Formula: C15H13Cl3O4

SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 363.62

Physical Properties

Property code	Value	Unit	Source
gf	-124.06	kJ/mol	Joback Method
hf	-401.01	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	84.18	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.287		Crippen Method
mcvol	241.450	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook
tb	838.77	K	Joback Method
tc	1067.32	K	Joback Method
tf	588.84	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.69	J/mol×K	838.77	Joback Method
cpg	621.10	J/mol×K	876.86	Joback Method
cpg	630.55	J/mol×K	914.95	Joback Method
cpg	639.05	J/mol×K	953.05	Joback Method
cpg	646.62	J/mol×K	991.14	Joback Method
cpg	653.27	J/mol×K	1029.23	Joback Method
cpg	659.01	J/mol×K	1067.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394006&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