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

Inchi: InChI=1S/C14H9Cl3O4/c1-3-8(2)20-12(18)4-5-13(19)21-14-10(16)6-9(15)7-11(14)17/h1,
InchiKey: OYOKCQOUIWZOIO-SNAWJCMRSA-N
Formula: C14H9Cl3O4
SMILES: C#CC(C)OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 347.58

Physical Properties

Property code	Value	Unit	Source
gf	-52.26	kJ/mol	Joback Method
hf	-263.15	kJ/mol	Joback Method
hfus	42.71	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.673		Crippen Method
mcvol	223.060	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
tb	820.05	K	Joback Method
tc	1059.44	K	Joback Method
tf	572.49	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.24	J/mol×K	820.05	Joback Method
cpg	539.66	J/mol×K	859.95	Joback Method
cpg	548.21	J/mol×K	899.85	Joback Method
cpg	555.94	J/mol×K	939.75	Joback Method
cpg	562.85	J/mol×K	979.64	Joback Method
cpg	568.99	J/mol×K	1019.54	Joback Method
cpg	574.38	J/mol×K	1059.44	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=U405948&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