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

Inchi: InChI=1S/C15H15Cl3O4/c1-3-9(2)21-13(19)5-4-6-14(20)22-15-11(17)7-10(16)8-12(15)18

InchiKey: RCMYEMACHAKHBA-UHFFFAOYSA-N

Formula: C15H15Cl3O4

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

Mol. weight [g/mol]: 365.64

Physical Properties

Property code	Value	Unit	Source
gf	-259.29	kJ/mol	Joback Method
hf	-567.48	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	83.66	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.840		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	845.33	K	Joback Method
tc	1066.87	K	Joback Method
tf	540.11	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.38	J/mol×K	845.33	Joback Method
cpg	683.04	J/mol×K	1029.95	Joback Method
cpg	676.03	J/mol×K	993.02	Joback Method
cpg	668.06	J/mol×K	956.10	Joback Method
cpg	659.14	J/mol×K	919.18	Joback Method
cpg	649.25	J/mol×K	882.25	Joback Method
cpg	689.12	J/mol×K	1066.87	Joback Method
dvisc	0.0000721	Pa×s	845.33	Joback Method

dvisc	0.0000893	Pa×s	794.46	Joback Method
dvisc	0.0001139	Pa×s	743.59	Joback Method
dvisc	0.0001505	Pa×s	692.72	Joback Method
dvisc	0.0002080	Pa×s	641.85	Joback Method
dvisc	0.0003038	Pa×s	590.98	Joback Method
dvisc	0.0004767	Pa×s	540.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405246&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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