Diglycolic acid, ethyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C12H11Cl3O5/c1-2-19-10(16)5-18-6-11(17)20-12-8(14)3-7(13)4-9(12)15/h3-4H

InchiKey: DGUZMZSNHKSTRQ-UHFFFAOYSA-N

Formula: C12H11Cl3O5

SMILES: CCOC(=O)COCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 341.57

Physical Properties

Property code	Value	Unit	Source
gf	-474.95	kJ/mol	Joback Method
hf	-757.93	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.132		Crippen Method
mcvol	213.650	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	802.87	K	Joback Method
tc	1023.63	K	Joback Method
tf	545.29	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.30	J/mol×K	802.87	Joback Method
cpg	567.19	J/mol×K	986.84	Joback Method
cpg	561.11	J/mol×K	950.05	Joback Method
cpg	554.06	J/mol×K	913.25	Joback Method
cpg	546.06	J/mol×K	876.46	Joback Method
cpg	537.13	J/mol×K	839.66	Joback Method
cpg	572.28	J/mol×K	1023.63	Joback Method
dvisc	0.0000838	Pa×s	802.87	Joback Method

dvisc	0.0001013	Pa×s	759.94	Joback Method
dvisc	0.0001253	Pa×s	717.01	Joback Method
dvisc	0.0001591	Pa×s	674.08	Joback Method
dvisc	0.0002088	Pa×s	631.15	Joback Method
dvisc	0.0002850	Pa×s	588.22	Joback Method
dvisc	0.0004087	Pa×s	545.29	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=U382731&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