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

Inchi: InChI=1S/C14H15Cl3O5/c1-2-3-4-21-12(18)7-20-8-13(19)22-14-10(16)5-9(15)6-11(14)17

InchiKey: ADAKUVKETHXTSS-UHFFFAOYSA-N

Formula: C14H15Cl3O5

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

Mol. weight [g/mol]: 369.62

Physical Properties

Property code	Value	Unit	Source
gf	-458.11	kJ/mol	Joback Method
hf	-799.21	kJ/mol	Joback Method
hfus	44.24	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.912		Crippen Method
mcvol	241.830	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2874.00		NIST Webbook
rinpol	2874.00		NIST Webbook
tb	848.63	K	Joback Method
tc	1065.41	K	Joback Method
tf	567.83	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.00	J/mol×K	848.63	Joback Method
cpg	677.40	J/mol×K	1029.28	Joback Method
cpg	671.01	J/mol×K	993.15	Joback Method
cpg	663.56	J/mol×K	957.02	Joback Method
cpg	655.07	J/mol×K	920.89	Joback Method
cpg	645.54	J/mol×K	884.76	Joback Method
cpg	682.72	J/mol×K	1065.41	Joback Method
dvisc	0.0000635	Pa×s	848.63	Joback Method

dvisc	0.0000774	Pa×s	801.83	Joback Method
dvisc	0.0000967	Pa×s	755.03	Joback Method
dvisc	0.0001244	Pa×s	708.23	Joback Method
dvisc	0.0001659	Pa×s	661.43	Joback Method
dvisc	0.0002312	Pa×s	614.63	Joback Method
dvisc	0.0003402	Pa×s	567.83	Joback Method

Sources

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=U382734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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