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

Inchi: InChI=1S/C15H17Cl3O5/c1-2-3-4-5-22-13(19)8-21-9-14(20)23-15-11(17)6-10(16)7-12(15

InchiKey: AVZPMORCLUOXFP-UHFFFAOYSA-N

Formula: C15H17Cl3O5

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

Mol. weight [g/mol]: 383.65

Physical Properties

Property code	Value	Unit	Source
gf	-449.69	kJ/mol	Joback Method
hf	-819.85	kJ/mol	Joback Method
hfus	46.83	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.302		Crippen Method
mcvol	255.920	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	871.51	K	Joback Method
tc	1087.28	K	Joback Method
tf	579.10	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.24	J/mol×K	871.51	Joback Method
cpg	701.05	J/mol×K	907.47	Joback Method
cpg	710.78	J/mol×K	943.43	Joback Method
cpg	719.43	J/mol×K	979.39	Joback Method
cpg	726.99	J/mol×K	1015.35	Joback Method
cpg	733.44	J/mol×K	1051.31	Joback Method
cpg	738.78	J/mol×K	1087.28	Joback Method
dvisc	0.0003085	Pa×s	579.10	Joback Method

dvisc	0.0002070	Pa×s	627.84	Joback Method
dvisc	0.0001472	Pa×s	676.57	Joback Method
dvisc	0.0001095	Pa×s	725.31	Joback Method
dvisc	0.0000846	Pa×s	774.04	Joback Method
dvisc	0.0000674	Pa×s	822.77	Joback Method
dvisc	0.0000550	Pa×s	871.51	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U382735&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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