Diglycolic acid, 4-chlorophenyl propyl ester

Inchi: InChI=1S/C13H15ClO5/c1-2-7-18-12(15)8-17-9-13(16)19-11-5-3-10(14)4-6-11/h3-6H,2,7

InchiKey: GFCAJEJEEJFGCI-UHFFFAOYSA-N

Formula: C13H15ClO5

SMILES: CCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 286.71

Physical Properties

Property code	Value	Unit	Source
gf	-423.41	kJ/mol	Joback Method
hf	-724.15	kJ/mol	Joback Method
hfus	34.04	kJ/mol	Joback Method
hvap	72.58	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.215		Crippen Method
mcvol	203.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	740.93	K	Joback Method
tc	951.16	K	Joback Method
tf	471.68	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.67	J/mol×K	740.93	Joback Method
cpg	551.27	J/mol×K	775.97	Joback Method
cpg	562.97	J/mol×K	811.01	Joback Method
cpg	573.76	J/mol×K	846.04	Joback Method
cpg	583.64	J/mol×K	881.08	Joback Method
cpg	592.60	J/mol×K	916.12	Joback Method
cpg	600.63	J/mol×K	951.16	Joback Method
dvisc	0.0006652	Pa×s	471.68	Joback Method

dvisc	0.0004162	Pa×s	516.56	Joback Method
dvisc	0.0002806	Pa×s	561.43	Joback Method
dvisc	0.0002006	Pa×s	606.31	Joback Method
dvisc	0.0001502	Pa×s	651.18	Joback Method
dvisc	0.0001167	Pa×s	696.06	Joback Method
dvisc	0.0000935	Pa×s	740.93	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=U381776&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