Diglycolic acid, 2,6-dimethoxyphenyl propyl ester

Inchi: InChI=1S/C15H20O7/c1-4-8-21-13(16)9-20-10-14(17)22-15-11(18-2)6-5-7-12(15)19-3/h5

InchiKey: SIXVHWZENADROY-UHFFFAOYSA-N

Formula: C15H20O7

SMILES: CCCOC(=O)COCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 312.32

Physical Properties

Property code	Value	Unit	Source
gf	-614.27	kJ/mol	Joback Method
hf	-1025.60	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.579		Crippen Method
mcvol	230.940	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2736.00		NIST Webbook
rinpol	2736.00		NIST Webbook
tb	799.08	K	Joback Method
tc	1001.34	K	Joback Method
tf	521.28	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.59	J/mol×K	799.08	Joback Method
cpg	688.18	J/mol×K	832.79	Joback Method
cpg	700.69	J/mol×K	866.50	Joback Method
cpg	712.11	J/mol×K	900.21	Joback Method
cpg	722.39	J/mol×K	933.92	Joback Method
cpg	731.51	J/mol×K	967.63	Joback Method
cpg	739.42	J/mol×K	1001.34	Joback Method
dvisc	0.0002967	Pa×s	521.28	Joback Method

dvisc	0.0001927	Pa×s	567.58	Joback Method
dvisc	0.0001336	Pa×s	613.88	Joback Method
dvisc	0.0000975	Pa×s	660.18	Joback Method
dvisc	0.0000742	Pa×s	706.48	Joback Method
dvisc	0.0000583	Pa×s	752.78	Joback Method
dvisc	0.0000472	Pa×s	799.08	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=U381903&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