Diglycolic acid, decyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C22H34O7/c1-4-5-6-7-8-9-10-11-15-28-20(23)16-27-17-21(24)29-22-18(25-2)1

InchiKey: AYGCNGDIAPBPTM-UHFFFAOYSA-N

Formula: C22H34O7

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

Mol. weight [g/mol]: 410.50

Physical Properties

Property code	Value	Unit	Source
gf	-555.33	kJ/mol	Joback Method
hf	-1170.08	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	93.71	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.310		Crippen Method
mcvol	329.570	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	3566.00		NIST Webbook
tb	959.24	K	Joback Method
tc	1174.41	K	Joback Method
tf	600.17	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.01	J/mol×K	959.24	Joback Method
cpg	1138.55	J/mol×K	1138.55	Joback Method
cpg	1131.19	J/mol×K	1102.69	Joback Method
cpg	1122.03	J/mol×K	1066.83	Joback Method
cpg	1111.11	J/mol×K	1030.96	Joback Method
cpg	1098.43	J/mol×K	995.10	Joback Method
cpg	1144.12	J/mol×K	1174.41	Joback Method
dvisc	0.0000172	Pa×s	959.24	Joback Method
dvisc	0.0000218	Pa×s	899.39	Joback Method

dvisc	0.0000286	Pa×s	839.55	Joback Method
dvisc	0.0000391	Pa×s	779.71	Joback Method
dvisc	0.0000563	Pa×s	719.86	Joback Method
dvisc	0.0000865	Pa×s	660.02	Joback Method
dvisc	0.0001449	Pa×s	600.17	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=U381912&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