Diglycolic acid, 2,6-dimethoxyphenyl pentyl ester

Inchi: InChI=1S/C17H24O7/c1-4-5-6-10-23-15(18)11-22-12-16(19)24-17-13(20-2)8-7-9-14(17)2

InchiKey: VZJFYFHJXZRHCS-UHFFFAOYSA-N

Formula: C17H24O7

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

Mol. weight [g/mol]: 340.37

Physical Properties

Property code	Value	Unit	Source
gf	-597.43	kJ/mol	Joback Method
hf	-1066.88	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	82.58	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.359		Crippen Method
mcvol	259.120	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2988.00		NIST Webbook
rinpol	2988.00		NIST Webbook
tb	844.84	K	Joback Method
tc	1046.96	K	Joback Method
tf	543.82	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.17	J/mol×K	844.84	Joback Method
cpg	802.16	J/mol×K	878.53	Joback Method
cpg	814.94	J/mol×K	912.21	Joback Method
cpg	826.47	J/mol×K	945.90	Joback Method
cpg	836.72	J/mol×K	979.59	Joback Method
cpg	845.68	J/mol×K	1013.27	Joback Method
cpg	853.30	J/mol×K	1046.96	Joback Method
dvisc	0.0002466	Pa×s	543.82	Joback Method

dvisc	0.0001561	Pa×s	593.99	Joback Method
dvisc	0.0001061	Pa×s	644.16	Joback Method
dvisc	0.0000762	Pa×s	694.33	Joback Method
dvisc	0.0000573	Pa×s	744.50	Joback Method
dvisc	0.0000446	Pa×s	794.67	Joback Method
dvisc	0.0000358	Pa×s	844.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381906&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

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

Latest version available from:
https://www.chemeo.com/cid/90-459-3/Diglycolic-acid-2-6-dimethoxyphenyl-pentyl-ester.pdf
Generated by Cheméo on 2024-05-03 09:18:20.687127183 +0000 UTC m=+17017149.607704495.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.