

Diglycolic acid, 2,6-dimethoxyphenyl ethyl ester

Inchi:	InChI=1S/C14H18O7/c1-4-20-12(15)8-19-9-13(16)21-14-10(17-2)6-5-7-11(14)18-3/h5-7H
InchiKey:	SEHPFIZSWVJLBI-UHFFFAOYSA-N
Formula:	C14H18O7
SMILES:	CCOC(=O)COCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	298.29

Physical Properties

Property code	Value	Unit	Source
gf	-622.69	kJ/mol	Joback Method
hf	-1004.96	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	75.90	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.189		Crippen Method
mvol	216.850	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	776.20	K	Joback Method
tc	979.47	K	Joback Method
tf	510.01	K	Joback Method
vc	0.814	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.16	J/molxK	776.20	Joback Method
cpg	675.34	J/molxK	945.59	Joback Method
cpg	666.25	J/molxK	911.71	Joback Method
cpg	656.04	J/molxK	877.83	Joback Method
cpg	644.77	J/molxK	843.96	Joback Method
cpg	632.46	J/molxK	810.08	Joback Method
cpg	683.29	J/molxK	979.47	Joback Method
dvisc	0.0000539	Paxs	776.20	Joback Method

dvisc	0.0000664	Paxs	731.84	Joback Method
dvisc	0.0000840	Paxs	687.47	Joback Method
dvisc	0.0001097	Paxs	643.11	Joback Method
dvisc	0.0001490	Paxs	598.74	Joback Method
dvisc	0.0002128	Paxs	554.38	Joback Method
dvisc	0.0003231	Paxs	510.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381902&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

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