

Diglycolic acid, 2,6-dimethoxyphenyl nonyl ester

Inchi:	InChI=1S/C21H32O7/c1-4-5-6-7-8-9-10-14-27-19(22)15-26-16-20(23)28-21-17(24-2)12-
InchiKey:	YNNSILGZZREMHY-UHFFFAOYSA-N
Formula:	C21H32O7
SMILES:	CCCCCCCCCOC(=O)COCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	396.47

Physical Properties

Property code	Value	Unit	Source
gf	-563.75	kJ/mol	Joback Method
hf	-1149.44	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	91.48	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.920		Crippen Method
mcvol	315.480	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
tb	936.36	K	Joback Method
tc	1147.16	K	Joback Method
tf	588.90	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.80	J/molxK	936.36	Joback Method
cpg	1038.18	J/molxK	971.49	Joback Method
cpg	1050.96	J/molxK	1006.63	Joback Method
cpg	1062.11	J/molxK	1041.76	Joback Method
cpg	1071.61	J/molxK	1076.89	Joback Method
cpg	1079.45	J/molxK	1112.02	Joback Method
cpg	1085.61	J/molxK	1147.16	Joback Method
dvisc	0.0001623	Paxs	588.90	Joback Method
dvisc	0.0000979	Paxs	646.81	Joback Method
dvisc	0.0000642	Paxs	704.72	Joback Method

dvisc	0.0000449	Paxs	762.63	Joback Method
dvisc	0.0000330	Paxs	820.54	Joback Method
dvisc	0.0000253	Paxs	878.45	Joback Method
dvisc	0.0000200	Paxs	936.36	Joback Method

Sources

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=U381911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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