Diglycolic acid, 4-methoxyphenyl nonyl ester

Inchi: InChI=1S/C20H30O6/c1-3-4-5-6-7-8-9-14-25-19(21)15-24-16-20(22)26-18-12-10-17(23-2
InchiKey: MEAWNARMMIAVMQ-UHFFFAOYSA-N
Formula: C20H30O6
SMILES: CCCCCCCCCOC(=O)COCC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
gf	-457.54	kJ/mol	Joback Method
hf	-985.11	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	86.18	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.911		Crippen Method
mcvol	295.520	ml/mol	McGowan Method
pc	1308.95	kPa	Joback Method
rinpol	3349.00		NIST Webbook
rinpol	3349.00		NIST Webbook
tb	886.08	K	Joback Method
tc	1089.73	K	Joback Method
tf	542.88	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.21	J/mol×K	886.08	Joback Method
cpg	951.30	J/mol×K	920.02	Joback Method
cpg	965.06	J/mol×K	953.96	Joback Method
cpg	977.51	J/mol×K	987.90	Joback Method
cpg	988.62	J/mol×K	1021.84	Joback Method
cpg	998.40	J/mol×K	1055.79	Joback Method
cpg	1006.86	J/mol×K	1089.73	Joback Method
dvisc	0.0002917	Pa×s	542.88	Joback Method

dvisc	0.0001676	Pa×s	600.08	Joback Method
dvisc	0.0001060	Pa×s	657.28	Joback Method
dvisc	0.0000722	Pa×s	714.48	Joback Method
dvisc	0.0000520	Pa×s	771.68	Joback Method
dvisc	0.0000392	Pa×s	828.88	Joback Method
dvisc	0.0000307	Pa×s	886.08	Joback Method

Sources

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=U381890&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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