Diglycolic acid, 4-methoxyphenyl octyl ester

Inchi: InChI=1S/C19H28O6/c1-3-4-5-6-7-8-13-24-18(20)14-23-15-19(21)25-17-11-9-16(22-2)10
InchiKey: RKYIHYKZYBJMLD-UHFFFAOYSA-N
Formula: C19H28O6
SMILES: CCCCCCCCOC(=O)COCC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]: 352.42

Physical Properties

Property code	Value	Unit	Source
gf	-465.96	kJ/mol	Joback Method
hf	-964.47	kJ/mol	Joback Method
hfus	46.57	kJ/mol	Joback Method
hvap	83.96	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.521		Crippen Method
mcvol	281.430	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	3236.00		NIST Webbook
rinpol	3236.00		NIST Webbook
tb	863.20	K	Joback Method
tc	1065.06	K	Joback Method
tf	531.61	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.07	J/mol×K	863.20	Joback Method
cpg	892.02	J/mol×K	896.84	Joback Method
cpg	905.71	J/mol×K	930.49	Joback Method
cpg	918.15	J/mol×K	964.13	Joback Method
cpg	929.33	J/mol×K	997.77	Joback Method
cpg	939.25	J/mol×K	1031.42	Joback Method
cpg	947.91	J/mol×K	1065.06	Joback Method
dvisc	0.0003244	Pa×s	531.61	Joback Method

dvisc	0.0001886	Pa×s	586.87	Joback Method
dvisc	0.0001203	Pa×s	642.14	Joback Method
dvisc	0.0000825	Pa×s	697.40	Joback Method
dvisc	0.0000597	Pa×s	752.67	Joback Method
dvisc	0.0000452	Pa×s	807.93	Joback Method
dvisc	0.0000355	Pa×s	863.20	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=U381889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume