Diglycolic acid, 4-methoxybenzyl pentyl ester

Inchi: InChI=1S/C17H24O6/c1-3-4-5-10-22-16(18)12-21-13-17(19)23-11-14-6-8-15(20-2)9-7-14
InchiKey: CEUBMSDIGXBWES-UHFFFAOYSA-N
Formula: C17H24O6
SMILES: CCCCCOC(=O)COCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-482.80	kJ/mol	Joback Method
hf	-923.19	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	79.51	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.488		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	3065.00		NIST Webbook
rinpol	3065.00		NIST Webbook
tb	817.44	K	Joback Method
tc	1017.95	K	Joback Method
tf	509.07	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.96	J/mol×K	817.44	Joback Method
cpg	775.54	J/mol×K	850.86	Joback Method
cpg	789.01	J/mol×K	884.28	Joback Method
cpg	801.34	J/mol×K	917.70	Joback Method
cpg	812.54	J/mol×K	951.12	Joback Method
cpg	822.59	J/mol×K	984.53	Joback Method
cpg	831.48	J/mol×K	1017.95	Joback Method
dvisc	0.0003963	Pa×s	509.07	Joback Method

dvisc	0.0002361	Pa×s	560.47	Joback Method
dvisc	0.0001535	Pa×s	611.86	Joback Method
dvisc	0.0001067	Pa×s	663.25	Joback Method
dvisc	0.0000781	Pa×s	714.65	Joback Method
dvisc	0.0000596	Pa×s	766.04	Joback Method
dvisc	0.0000471	Pa×s	817.44	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=U382249&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