Diglycolic acid, isobutyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C17H24O6/c1-12(2)9-21-16(18)10-20-11-17(19)23-15-8-6-5-7-14(15)22-13(3)4

InchiKey: BTIOTMSPINGVQU-UHFFFAOYSA-N

Formula: C17H24O6

SMILES: CC(C)COC(=O)COCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-487.68	kJ/mol	Joback Method
hf	-933.75	kJ/mol	Joback Method
hfus	34.34	kJ/mol	Joback Method
hvap	78.73	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.595		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
tb	816.56	K	Joback Method
tc	1021.49	K	Joback Method
tf	479.07	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.06	J/mol×K	816.56	Joback Method
cpg	776.94	J/mol×K	850.71	Joback Method
cpg	790.64	J/mol×K	884.87	Joback Method
cpg	803.14	J/mol×K	919.02	Joback Method
cpg	814.43	J/mol×K	953.18	Joback Method
cpg	824.50	J/mol×K	987.33	Joback Method
cpg	833.34	J/mol×K	1021.49	Joback Method
dvisc	0.0005055	Pa×s	479.07	Joback Method

dvisc	0.0002647	Pa×s	535.32	Joback Method
dvisc	0.0001568	Pa×s	591.57	Joback Method
dvisc	0.0001017	Pa×s	647.82	Joback Method
dvisc	0.0000707	Pa×s	704.06	Joback Method
dvisc	0.0000518	Pa×s	760.31	Joback Method
dvisc	0.0000397	Pa×s	816.56	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=U381980&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